Neutrons for Quantum Magnetism

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Outline

Conventional Magnets

Long-range magnetic order and spin-wave excitations

Origins of Quantum magnetism

low spin values, antiferromagnetic, low-dimensional, frustration, spin liquids

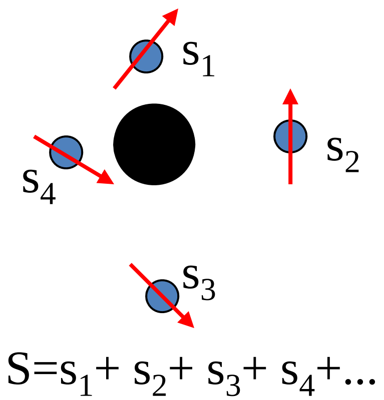
Neutron scattering for quantum magnets

Triple Axis spectrometer, time-of-flight spectrometer

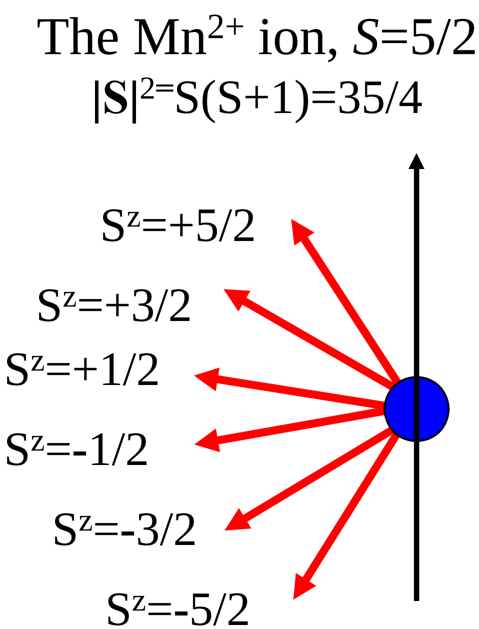
Examples of frustrated magnets

0-dimensional magnets e.g. dimer magnets
1.Dimensional magnets e.g. the spin-1/2 chain
2-Dimensional magnets e.g. Square, triangular, kagome, lattice
3-Dimensional magnets e.g. pyrochlore, spin ice and water ice

Conventional Magnetism – Magnetic Moments



- Electrons possess spin and orbital angular momenta (*s* and ***l***).
- ***S*** and ***L*** for an ion can be determined by summing the electronic ***s*** and ***l*** of the unpaired electrons
- The ionic magnetic moment is $\boldsymbol{m}=g_s\mu_B\boldsymbol{S}$.



- *S* is the quantum number associated with the angular momentum ***S***.
- *S* is restricted to take on discrete values either integer or half integer.

Conventional Magnetism - Exchange Interactions

Heisenberg interactions

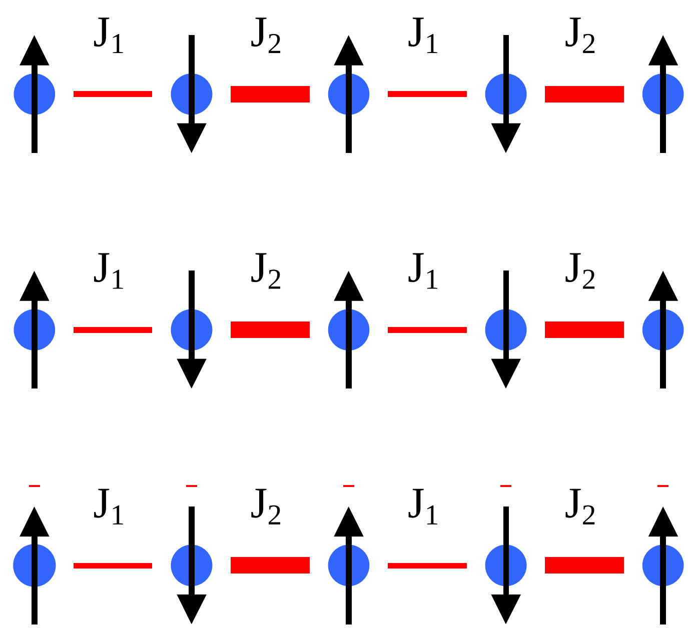
$$H = \sum_{n,m} J_{n,m} \mathbf{S}_n . \mathbf{S}_m$$

J < 0 ferromagnetic
J > 0 antiferromagnetic

3D magnet

$|J_1|=|J_2|=|J_3|=|J_4|$

e.g. $RbMnF_3$



1D magnet

$|J_1|=|J_2|$, $J_3=J_4=0$

e.g. $KCuF_3$

2D magnet

$|J_1|=|J_2|=|J_3|$, $J_4=0$

e.g. La_2CuO_4 and CFTD

1D alternating magnet

$|J_1|\neq|J_2|$, $J_3=J_4=0$

e.g. $CuGeO_3$ and $CuWO_4$

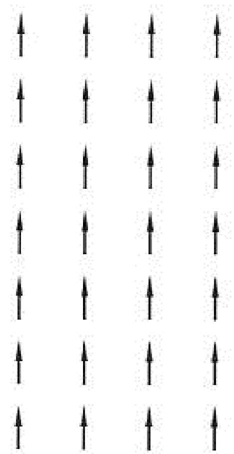
Anisotropic interactions

$$H = \sum_{n,m} -J_{n,m} \left[\varepsilon \left(\mathbf{S}_n^x \mathbf{S}_m^x + \mathbf{S}_n^y \mathbf{S}_m^y \right) + \mathbf{S}_n^z \mathbf{S}_m^z \right]$$

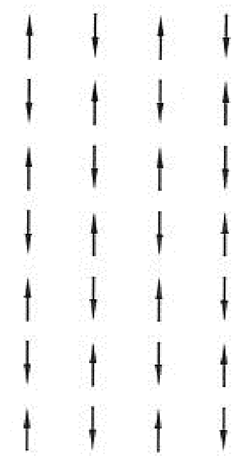
Conventional Magnetism - Ordered Ground State

Exchange interactions between magnetic ions often lead to long-range order in the ground state.

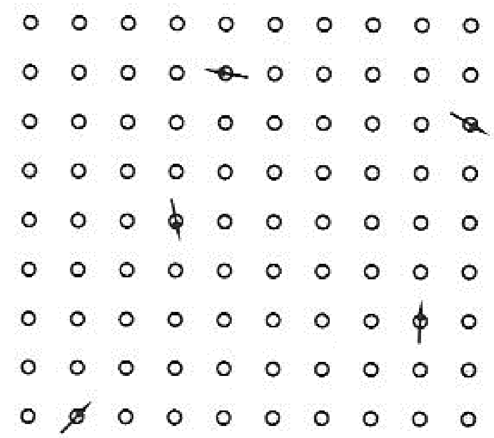
ferromagnet



antiferromagnet



spin glass



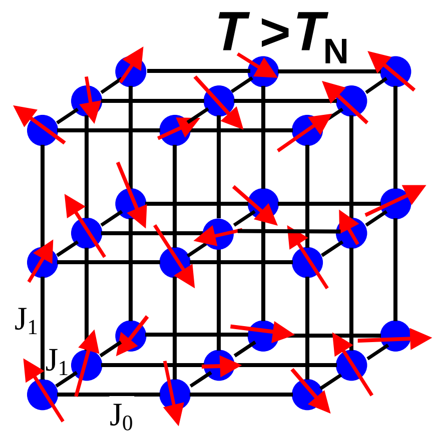
spiral magnet

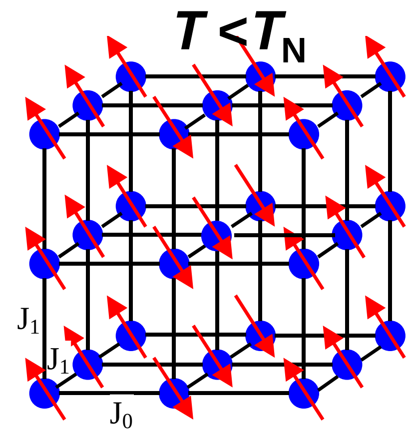
helical magnet

Conventional Antiferromagnets

Real Space

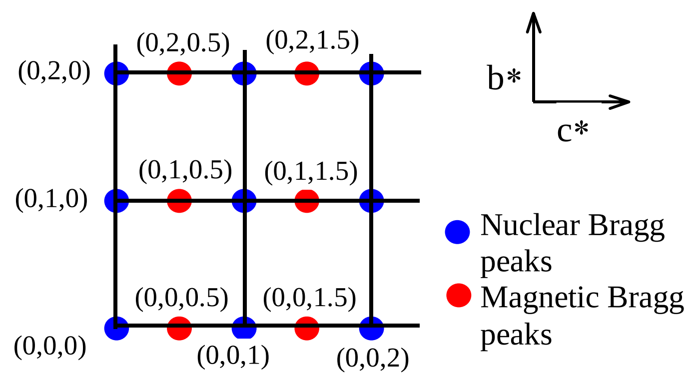
- Long-range magnetic order on cooling as thermal fluctuations weaken

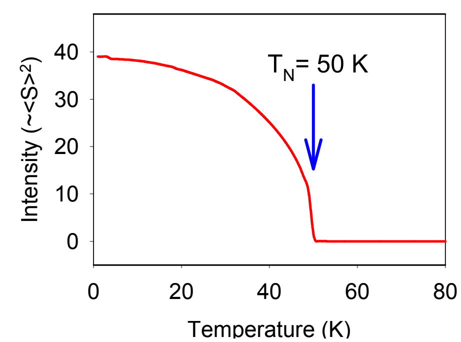




Reciprocal Space

- Magnetic Bragg peaks appear below the transition temperatures and grow as a function of temperature





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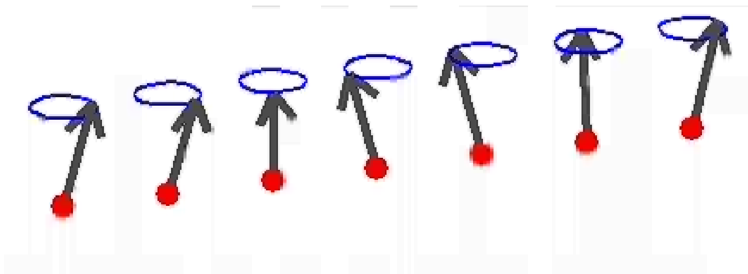
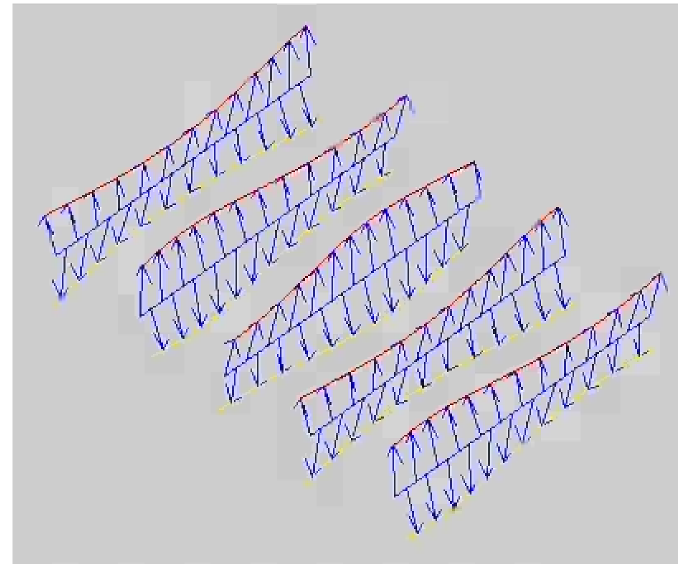
Magnetic Excitations

Real Space

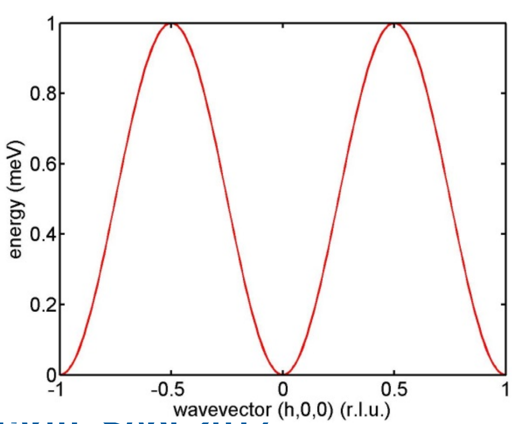
- Spin-waves are the collective motion of spins, about an ordered ground state (similar to phonons)

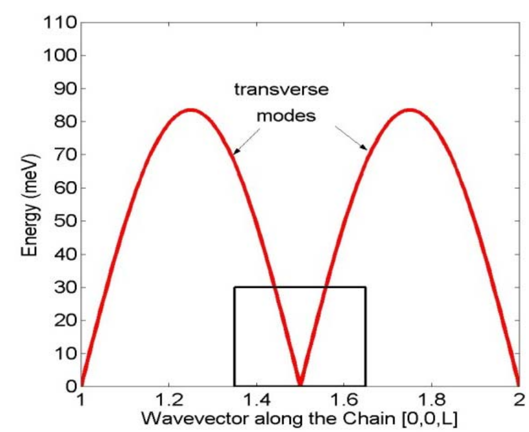




Reciprocal Space

- Observed as a well defined dispersion in energy and wavevector





The Origins of Quantum Magnetism

- Quantum fluctuations suppress long-range magnetic order, spin-wave theory fails
- Quantum effects are most visible in magnets with
  - low spin values
  - antiferromagnetic exchange interactions
  - low-dimensional interactions
  - frustrated interactions
- Quantum effects give rise to exotic states and excitations

$$H = \sum_{n,m \neq n} H_{n,m}$$

$$H_{n,m} = J_{n,m} \mathbf{S}_n \mathbf{S}_m = J_{n,m} \left(S_n^x S_m^x + S_n^y S_m^y + S_n^z S_m^z \right)$$

$$H_{n,m} = \boxed{J_{n,m} S_n^z S_m^z} + \boxed{J \left(S_n^+ S_m^- + S_n^- S_m^+ \right)}$$

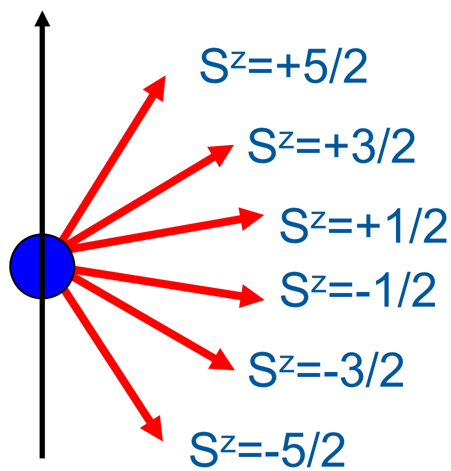
Quantum Magnetism - Low Spin Value

$$H_{n,m} = J_{n,m} S_n^z S_m^z + J\left(S_n^+ S_m^- + S_n^- S_m^+\right)$$

- Fluctuations have the largest effect for low spin values
- For S=1/2, changing S^z by 1 unit reverses the spin direction

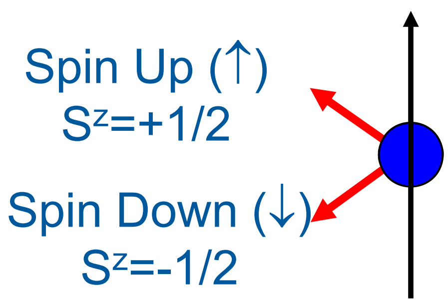
S=5/2

|S|^{2}=S(S+1)=35/4

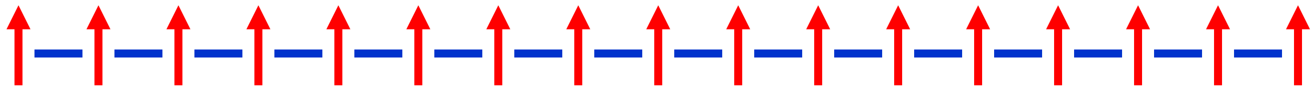


S=1/2

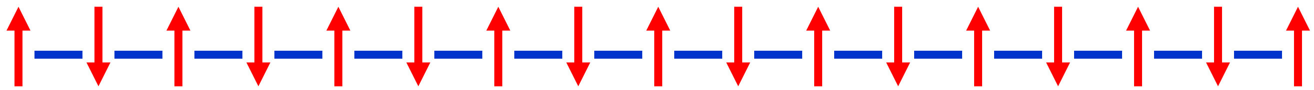
|S|^{2}=S(S+1)=3/4



Antiferromagnetic Exchange Interactions

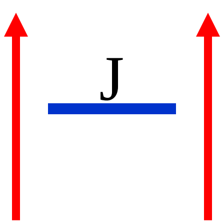


- Parallel spin alignment is an eigenstate of the Hamiltonian and the ground state of a ferromagnet.



- Antiparallel spin alignment (Néel state) is not an eigenstate of the Hamiltonain and is not the true ground state of an antiferromagnet.

J>0
ferromagnetic



S_1=1/2 S^z=1/2

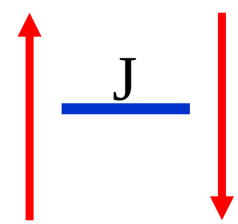
S_2=1/2 S^z=1/2

$$H_{1,2} = J\left(S_1^+ S_2^- + S_1^- S_2^+ + S_1^z S_2^z\right)$$

$$H_{1,2}\left|\uparrow_1 \uparrow_2\right\rangle = J/4\left|\uparrow_1 \uparrow_2\right\rangle$$

$$H_{1,2}\left|\uparrow_1 \downarrow_2\right\rangle = -J/4\left|\uparrow_1 \downarrow_2\right\rangle + J/4\left|\downarrow_1 \uparrow_2\right\rangle$$

J>0
antiferromagnetic



S_1=1/2 S^z=1/2

S_2=1/2 S^z=-1/2

Low-Dimensional Interactions

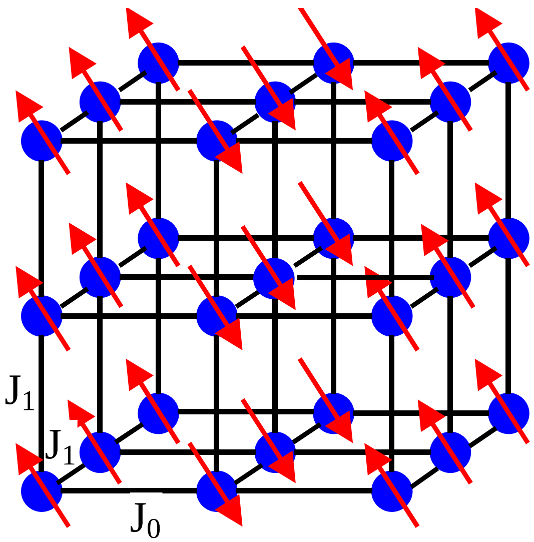
For three-dimensional magnets each magnetic ion has six neighbours

For a one-dimensional magnet there are only two neighbours

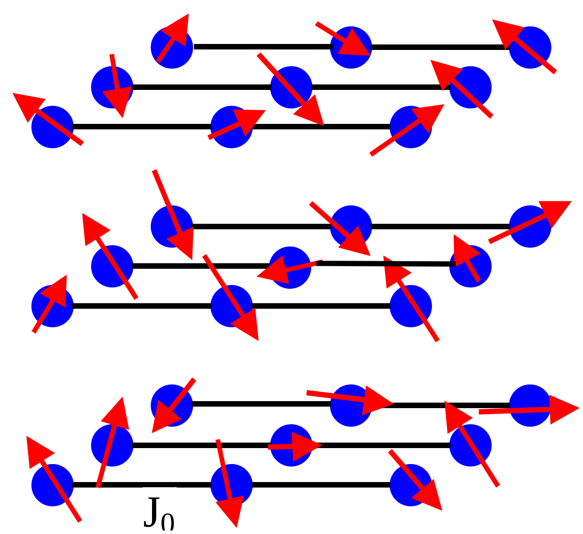
Neighbouring ions stabilize long-range order and reduce fluctuations

$$H_{n,m} = J_{n,m} S_n^z S_m^z + J\left(S_n^+ S_m^- + S_n^- S_m^+\right)$$

3D S=1/2

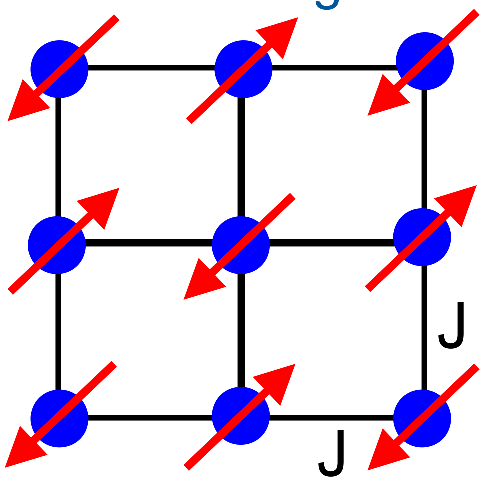


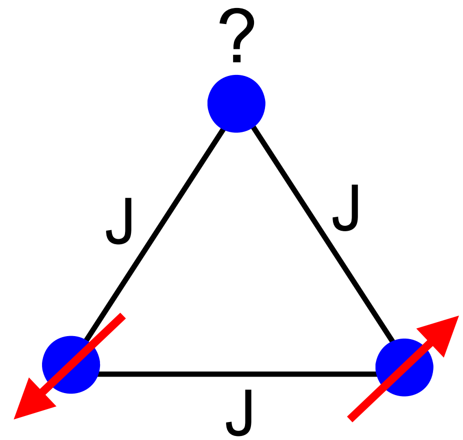
1D S=1/2



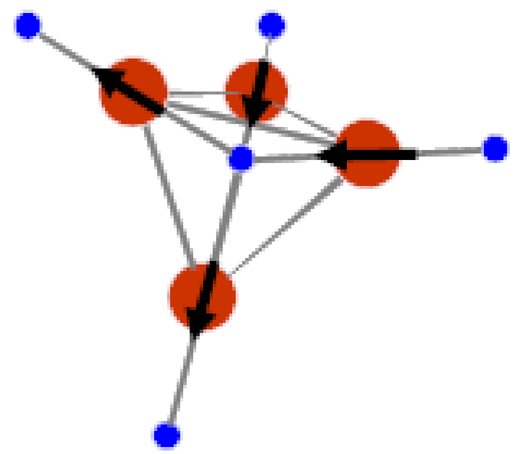
Frustrated Interactions

- In some lattices with antiferromagnetic interactions it is impossible for the spins to satisfy all the bonds simultaneously, this phenomenon is known as a geometrical frustration.
- Long-range order is suppressed as the spins fluctuate between the different degenerate configurations.





Anisotropy produces frustration if the anisotropy is incompatible with the spin direction favoured by the interactions



Examples of Quantum Magnets

- Quantum magnets are characterised by suppression of magnetic order, $T_N << T_{CW}$ and $<S> < S$, in some cases the magnet never orders.

- The excitations are broadened and renormalised with respect to spin-wave theory, and can be characterised by different quantum numbers.
- New theoretical approaches are required to understand these systems

Spin liquids,

- no local order, no static magnetism
  highly entangled, dynamic ground state,
  topological order, spinon excitations

Neutron Scattering for Quantum Magnets

Magnetic order is suppressed therefore most information about quantum magnets comes from their excitations.

It is important to resolve the excitations as a function of energy

- inelastic neutron scattering.

Since the excitations are often diffuse

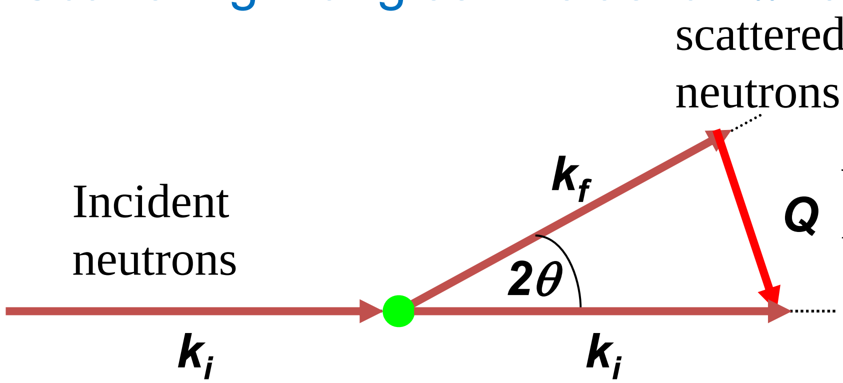
– wide detector coverage is useful

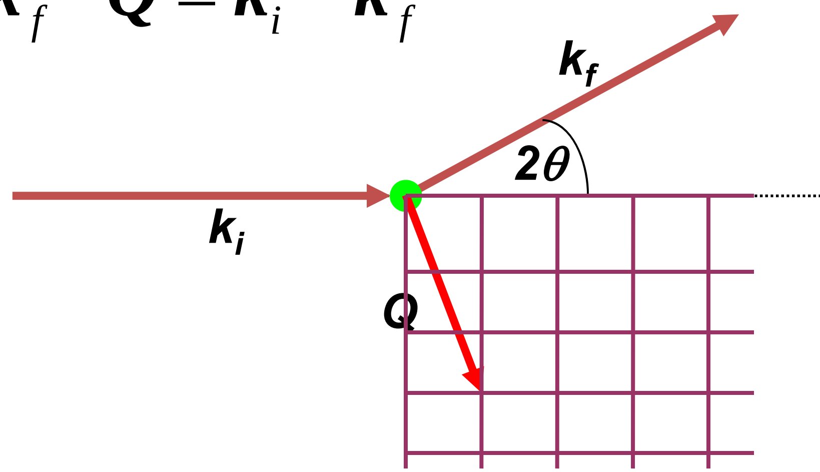
Conservation Laws and Scattering Triangles

Conservation of energy $$\hbar\omega = E_i - E_f = \frac{1}{2}mv_i^2 - \frac{1}{2}mv_f^2 = \frac{1}{2m}\hbar^2\left(k_i^2 - k_f^2\right)$$

Conservation of momentum $$\hbar\mathbf{Q} = \hbar\mathbf{k}_i - \hbar\mathbf{k}_f \qquad \mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

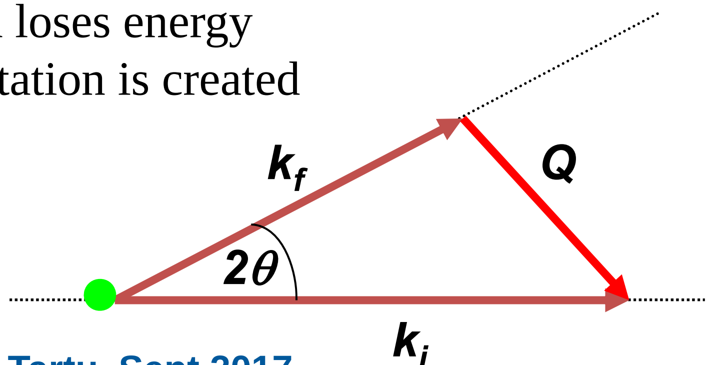
Scattering triangles - elastic $\hbar\omega=0$; $|k_i| = |k_f|$



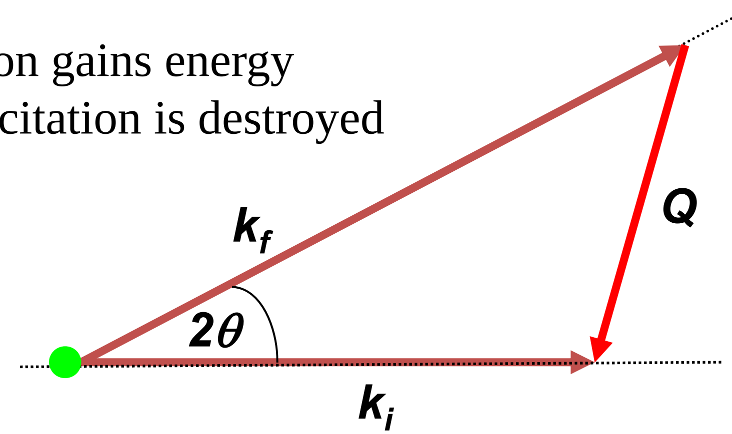


Scattering triangles - Inelastic $\hbar\omega \neq 0$; $|k_i| \neq |k_f|$

Neutron loses energy
An excitation is created



Neutron gains energy
An excitation is destroyed



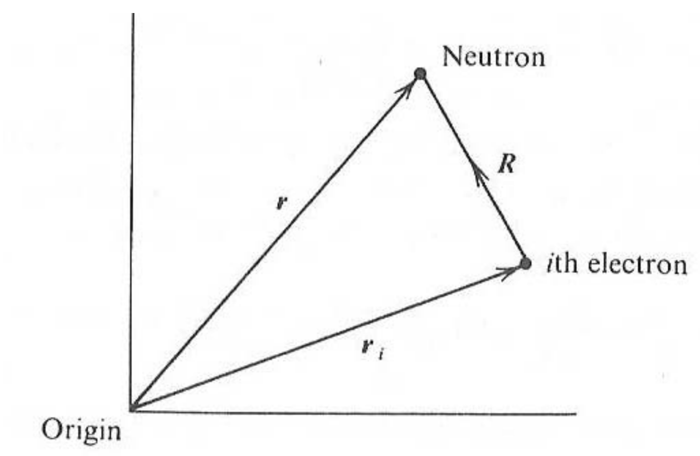
The Magnetic Cross-section

$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\left(\frac{m}{2\pi\hbar^2}\right)^2 \sum_{\rho_i, s_i} p_{\lambda_i} p_{s_i} \sum_{\rho_f, s_f} \left|\left\langle \boldsymbol{k}_f s_f \rho_f \left| V \right| \boldsymbol{k}_i s_i \rho_i \right\rangle\right|^2 \delta\left(E_{\rho_i} - E_{\rho_f} + \hbar\omega\right) \qquad E = \hbar\omega = \frac{\hbar^2}{2m}\left(k_i^2 - k_f^2\right)$$

V - the magnetic interaction between neutron and electrons

The electrons in an atom possess spin and orbital angular momentum, both of which give rise to an effective magnetic field. The neutrons interact with this field because they possess a spin moment

The interaction between a neutron at point **R** away from an electron with momentum ***l*** and spin ***s*** is



$$V_{magnetic} = -\boldsymbol{\mu}_n.\boldsymbol{B} = \frac{-\mu_0\gamma\mu_N 2\mu_B}{4\pi}\sum_j \boldsymbol{\sigma}.\left\{curl\left(\frac{\boldsymbol{s}_j \times \hat{\boldsymbol{R}}_j}{R^2}\right) + \frac{1}{\hbar}\left(\frac{\boldsymbol{l}_j \times \hat{\boldsymbol{R}}_j}{R^2}\right)\right\}$$

$$V_{nuclear} = \frac{2\pi\hbar}{m}\sum_j b_j \delta\left(\boldsymbol{r} - \boldsymbol{r}_j\right)$$

The Magnetic Cross-section

Cross section for spin only scattering by ions

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right) = \frac{(\gamma r_0)^2}{2\pi\hbar}\frac{k_f}{k_i}\left[F(\mathbf{Q})\right]^2 \exp\langle -2W\rangle \sum_{\alpha,\beta}\left(\delta_{\alpha,\beta} - \hat{Q}_\alpha \hat{Q}_\beta\right) S^{\alpha\beta}(\mathbf{Q},\omega)$$

$$S^{\alpha\beta}(\mathbf{Q},\omega) = \sum_{r_i}\sum_{r_j}\exp\left(i\mathbf{Q}.\left(\boldsymbol{r}_i - r_j\right)\right)\int_{-\infty}^{\infty}\left\langle S_{r_i}^{\alpha}(0)\, S_{r_j}^{\beta}(t)\right\rangle \exp(i\omega t)\, dt$$

For elastic neutron scattering it becomes

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{(\gamma r_0)^2}{2\pi\hbar}\frac{k_f}{k_i}\left[F(\mathbf{Q})\right]^2 \exp\langle -2W\rangle \sum_{\alpha,\beta}\left(\delta_{\alpha,\beta} - \hat{Q}_\alpha \hat{Q}_\beta\right)\sum_{r_i}\sum_{r_j}\exp\left(i\mathbf{Q}.\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right)\right)\left\langle S_{r_i}^{\alpha} S_{r_j}^{\beta}\right\rangle$$

$F(\mathbf{Q})$ Magnetic form factor which reduces intensity with increasing wavevector

exp<-2*W*> Debye-Waller factor which reduces intensity with increasing temperature

$\left(\delta_{\alpha,\beta} - \hat{Q}_\alpha \hat{Q}_\beta\right)$ polarisation factor which ensures only components of spin perpendicular to Q are observed

$\left\langle S_{r_i}^{\alpha}(0)\, S_{r_j}^{\beta}(t)\right\rangle$ is the spin-spin correlation function which describes how two spins separated in distance and time a related

Distinguishing Phonons and Magnons with Neutrons

Wavevector-dependence

- Structural excitations have high intensity at large |Q| and when **Q** is parallel to the mode of vibration
- Magnetic excitations have high intensity at low |Q| and when **Q** is perpendicular to the magnetic moment direction

Temperature dependence

- Structural excitations become stronger as temperature increases
- Magnetic excitations become weaker as temperature increases

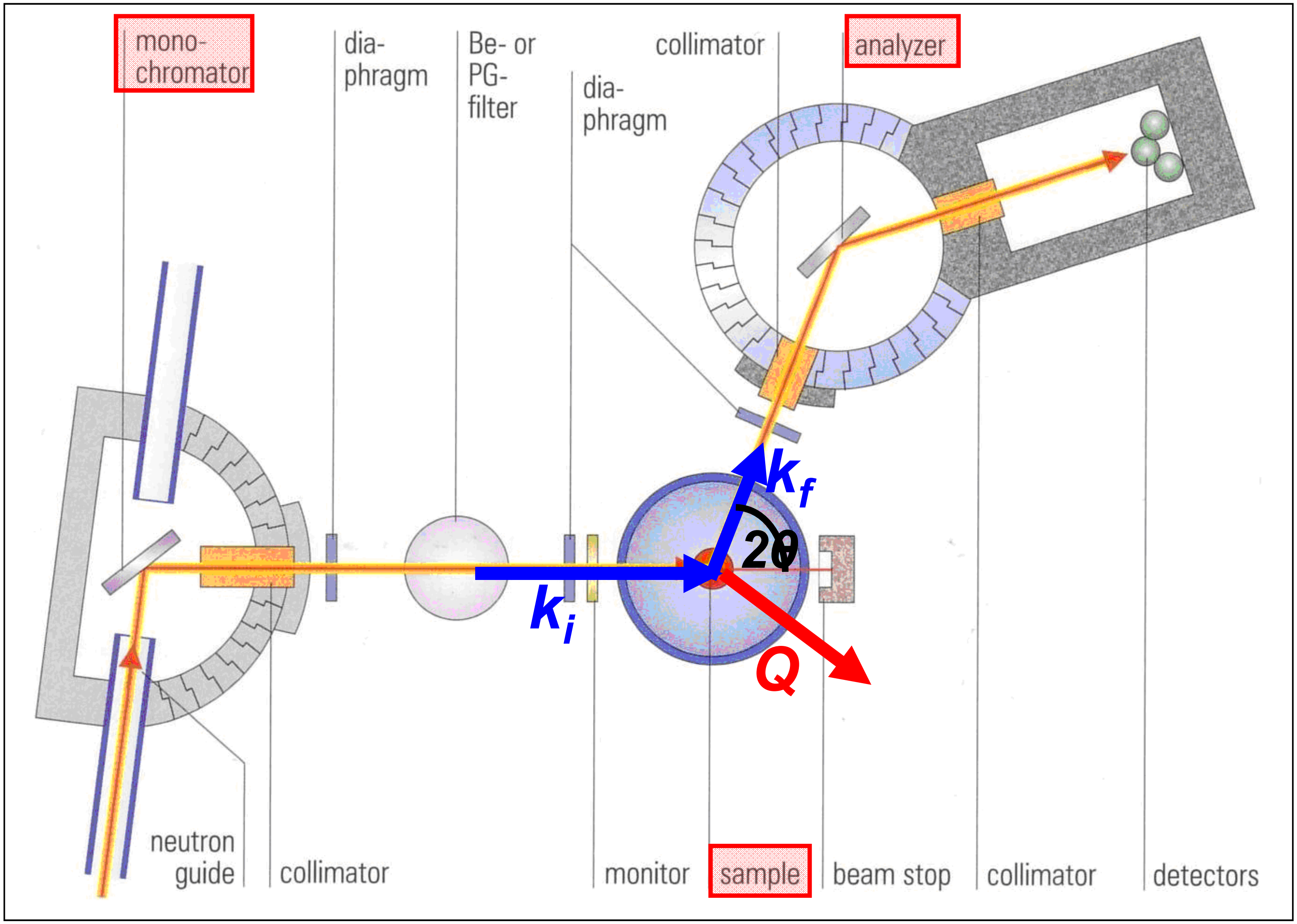
Instruments for Measuring Inelastic Scattering

Inelastic neutron scattering
- both the initial and final neutron energy

Triple-axis spectrometer
The initial and final neutron energies can be selected or measured using monochromator and analyser crystals where the wavelength of the neutrons is determined by the scattering angle.

Time-of-flight Spectrometer.
The initial and final energies are selected or measured using the time it takes the neutron to travel through spectrometer to the detector from this the velocity and hence kinetic energy are deduced.

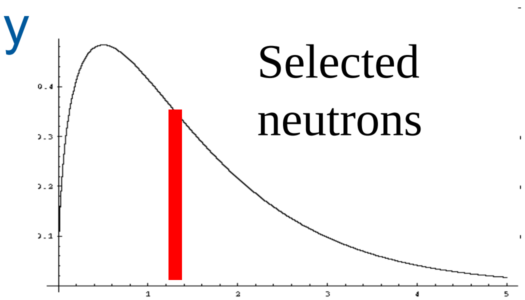
The Triple Axis Spectrometer - Layout



The Triple Axis Spectrometer – Monochromator Analyser

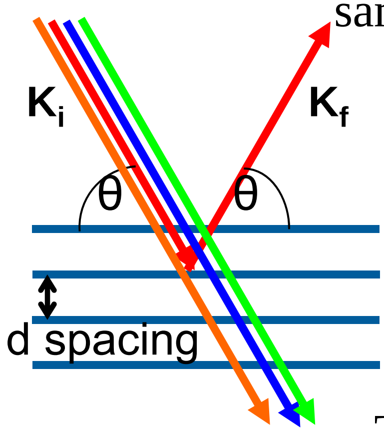
The monochromator is a crystalline material and selects a single wavelength from the white neutron beam of the reactor/spallation source by Bragg scattering where the scattering angle is chosen to select λ. The analyser measures the final neutron energy

$2d \sin\theta = n\lambda$
$n = 1,2,3\ldots.$



Incident white neutron beam

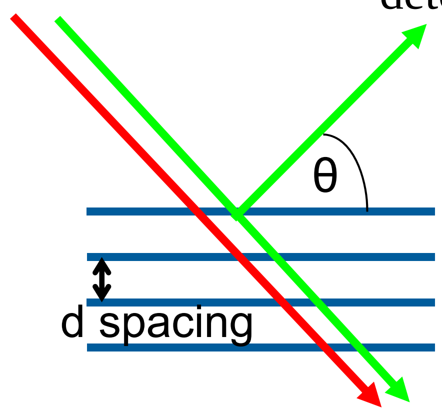
Diffracted Neutrons to sample



Transmitted neutrons

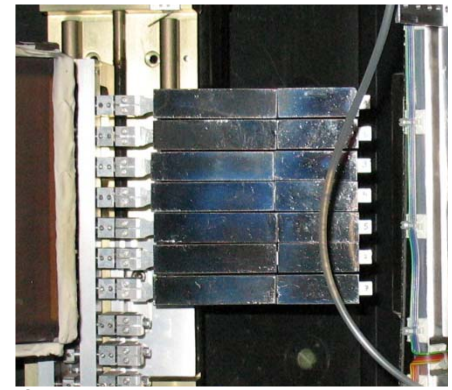
neutron beam scattered by the sample

Diffracted Neutrons to the detector



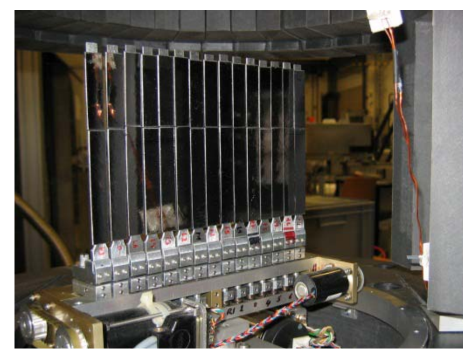
Transmitted neutrons

Vertically focusing monochromator

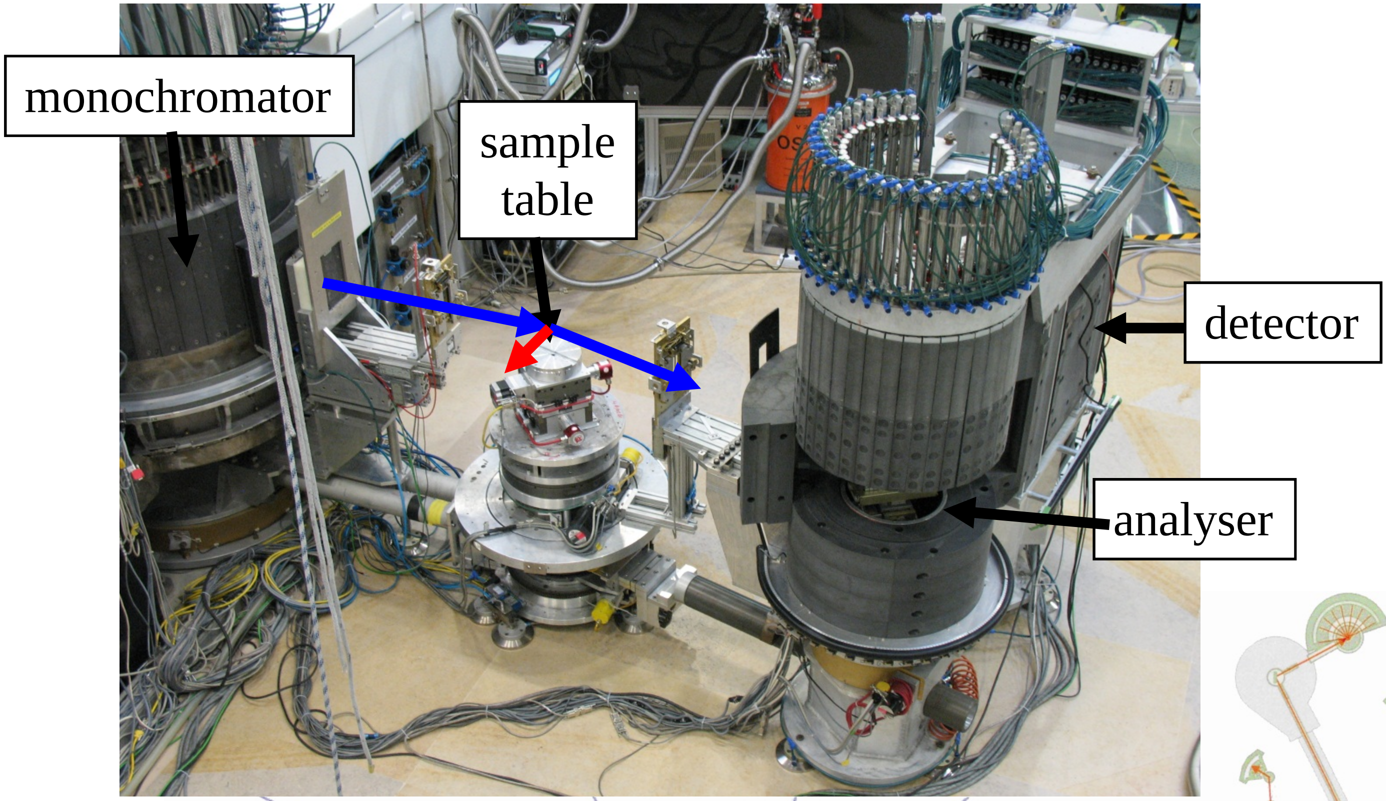


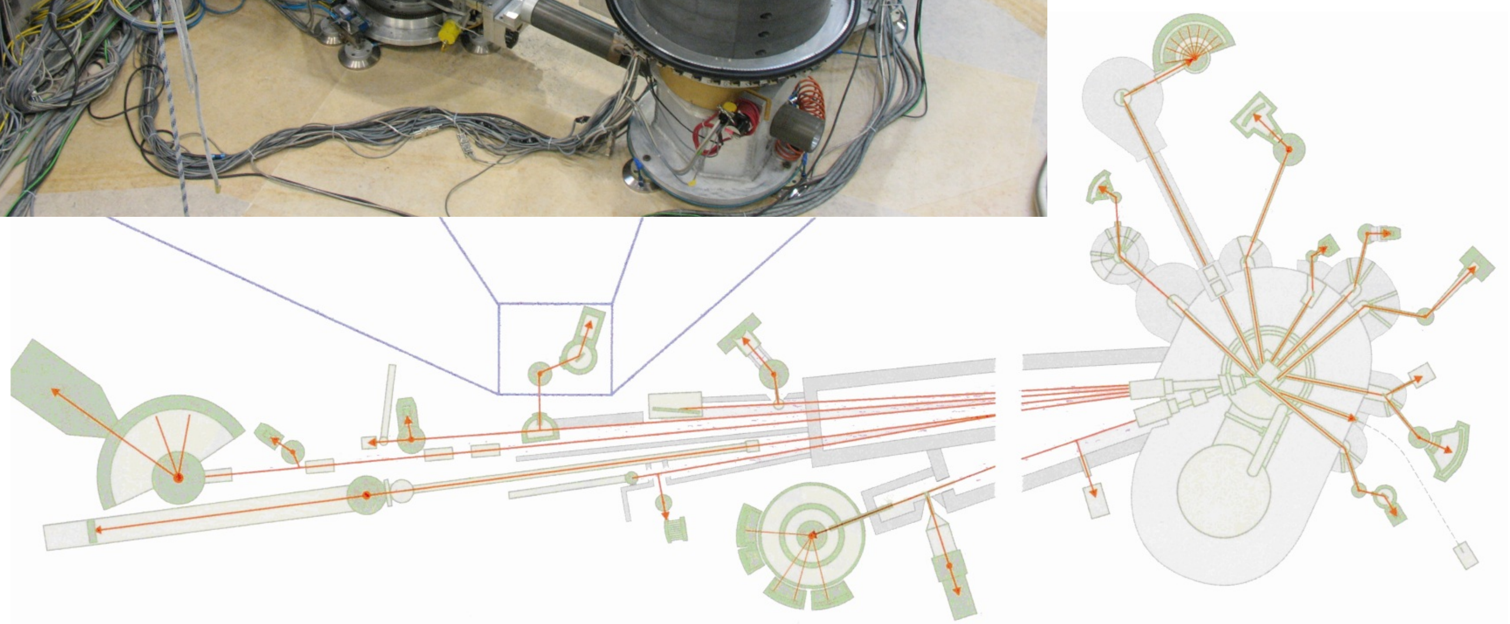
from graphite, Copper, Germanium, blades can be focused

Horizontally focusing monochromator



The Triple Axis Spectrometer – V2/FLEX, HZB

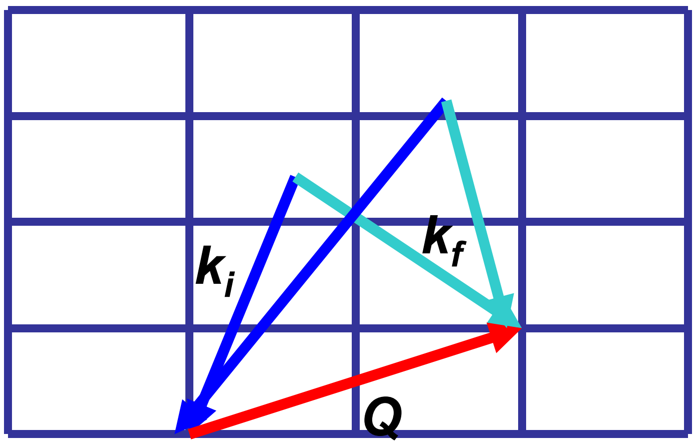


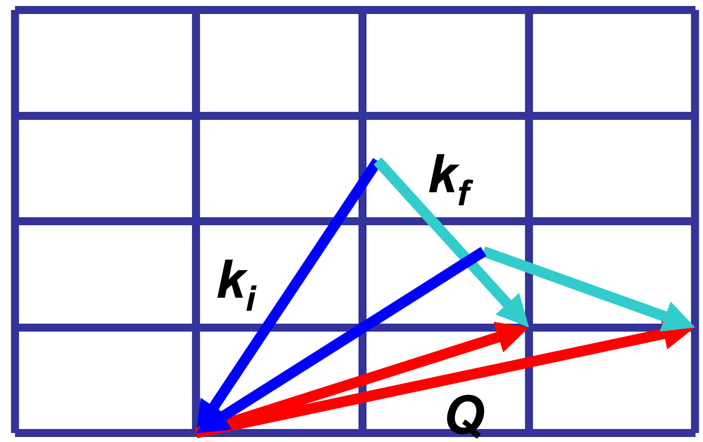


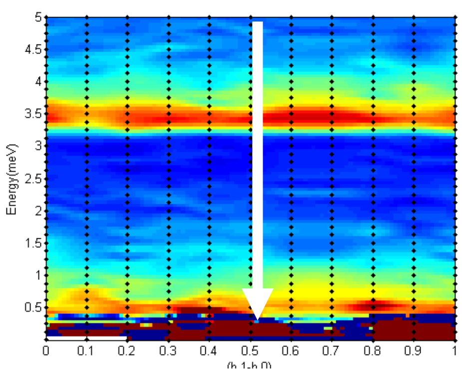
The Triple Axis Spectrometer – Measurements

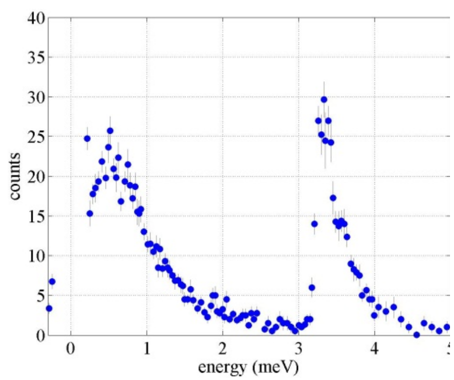
Keep wavevector transfer constant and, scan energy transfer.

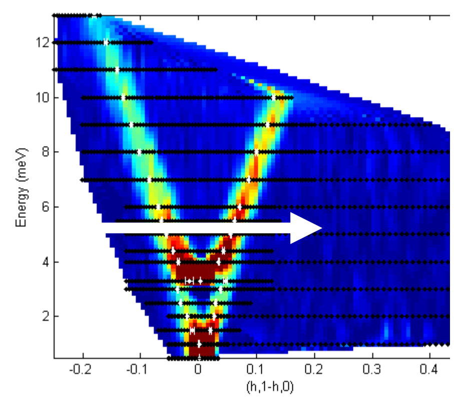
Keep energy transfer constant and, scan wavevector transfer.

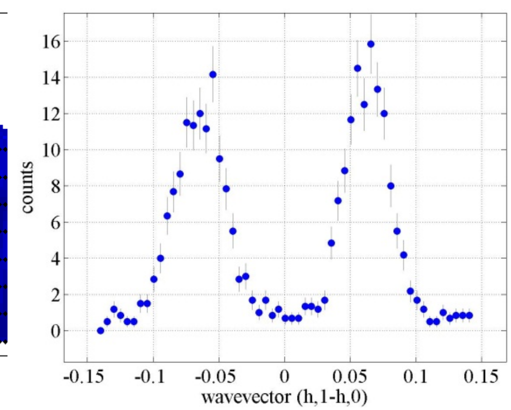












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Triple Axis Spectrometer – Pros and Cons

Advantages

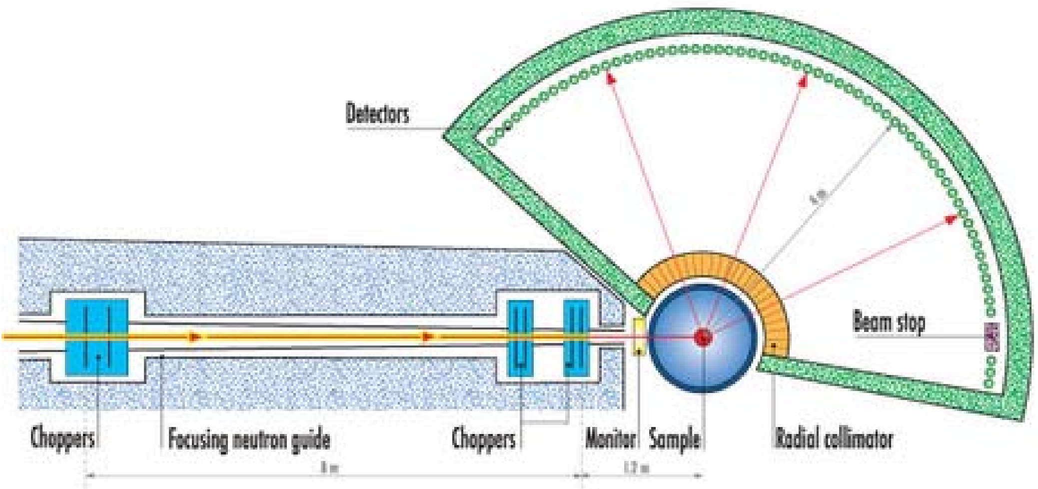
- Can focus all intensity on a specific point in reciprocal space
- Can make measurements along high-symmetry directions
- Can use focusing and other ‘tricks’ to improve the signal/noise ratio
- Can use polarisation analysis to separate magnetic and phonon signals

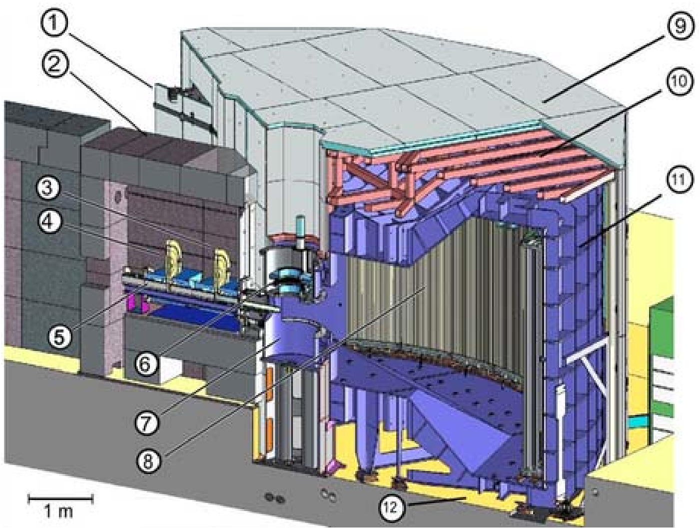
Disadvantages

- Technique is slow and requires some expert knowledge
- Use of monochromator and analyser crystals gives rise to possible higher-order effects that are known as “spurions”
- With measurements restricted to high-symmetry directions it is possible that something important might be missed

Time of Flight Spectrometer – Layout of V3/NEAT

Time and distance are used to calculate the initial and final neutron velocity and therefore energy. This is achieved by cutting the incident beam into pulses to give an initial time and incident energy





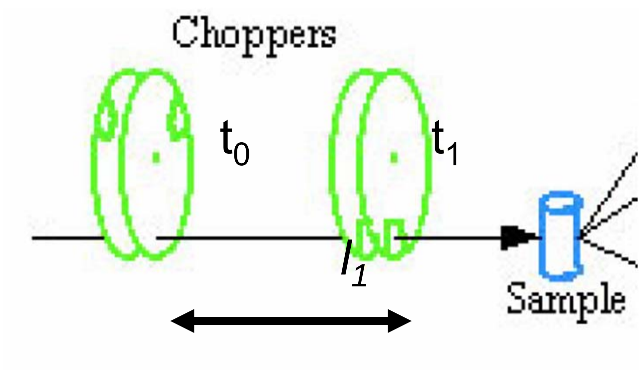
IN5, ILL

Time of Flight Spectrometer - Choppers

The neutron beam is cut into pulses of neutrons using disk choppers.

Ist chopper spins letts neutrons through once per revolution and sets initial time t_0

2nd chopper spins at the same rate and opens at a specific time later. The phase is chosen to select neutrons of a specific velocity and energy.



$$v_i = \frac{l_1}{(t_1 - t_0)}$$

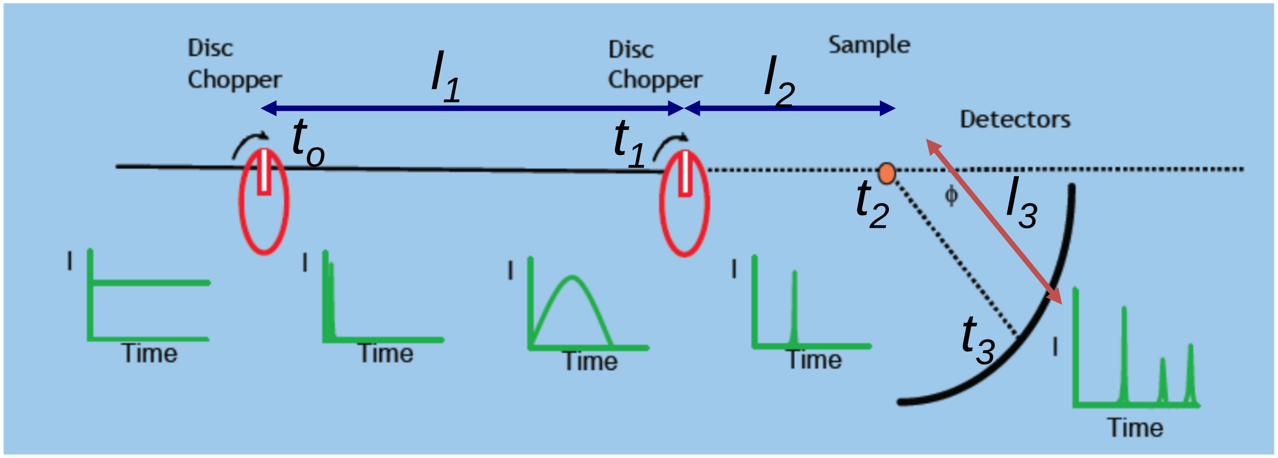
$$E_i = \frac{mv^2}{2} = \frac{ml_1^2}{2(t_1 - t_0)^2}$$

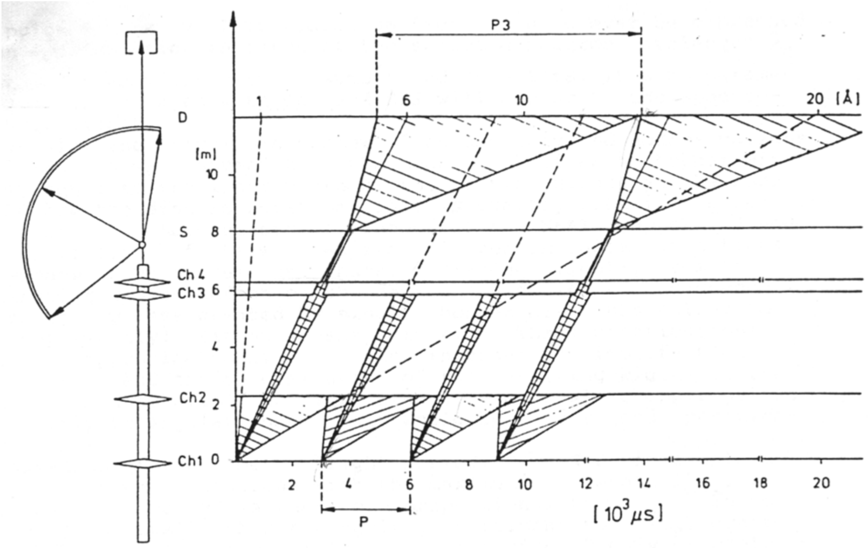
After scattering at the sample the detector again measures time as well as number of neutrons, thus the velocity and energy of the scattered neutrons is known.

The Time of Flight Spectrometer - Choppers

$$E_i = \frac{ml_1^2}{2(t_1 - t_0)^2}$$

$$E_f = \frac{m(l_3)^2}{2(t_3 - t_2)^2}$$





- First chopper sets the initial time.
- Second chopper sets the initial energy
- Detectors measure final time and energy.

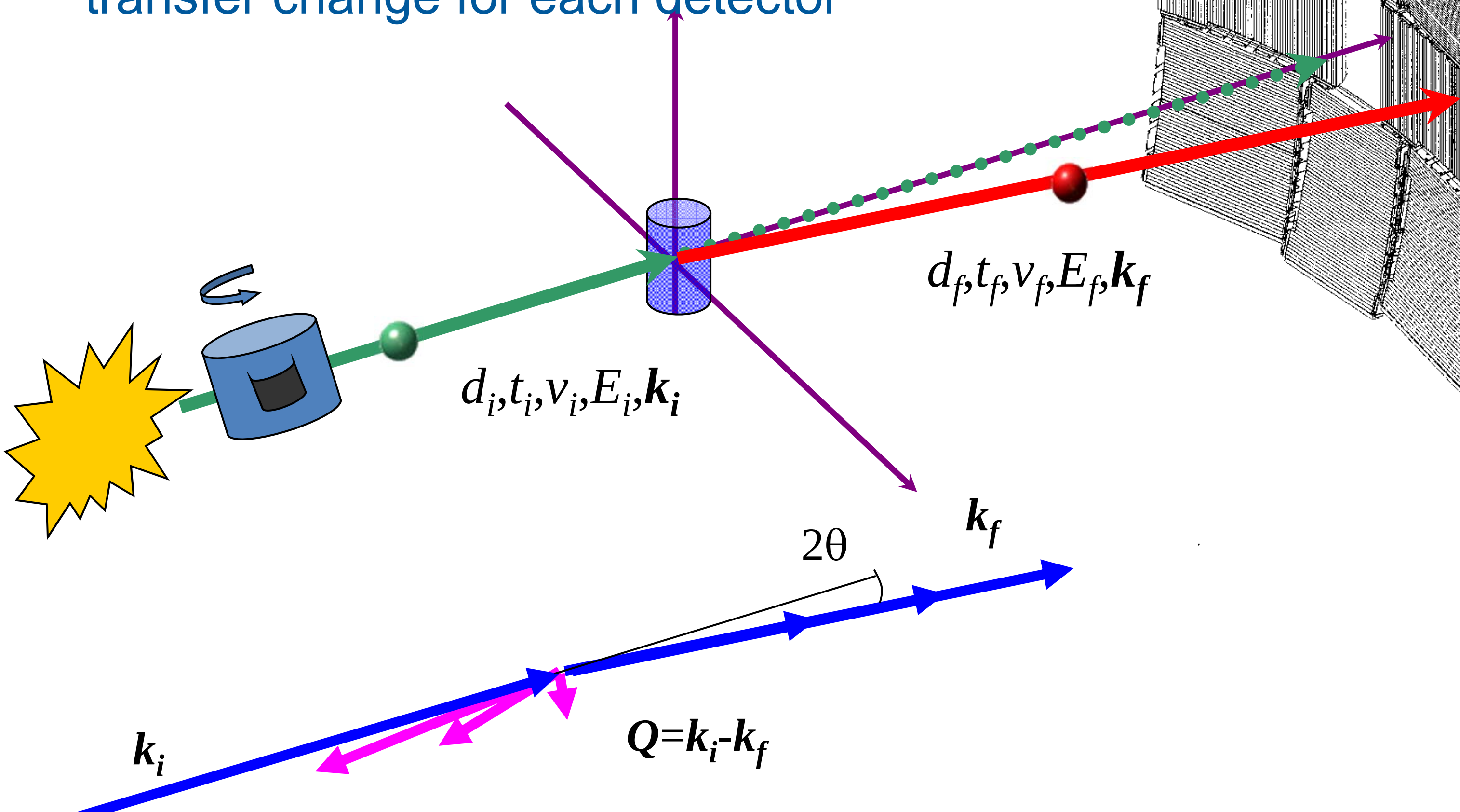
Time of Flight Spectrometer – Detectors

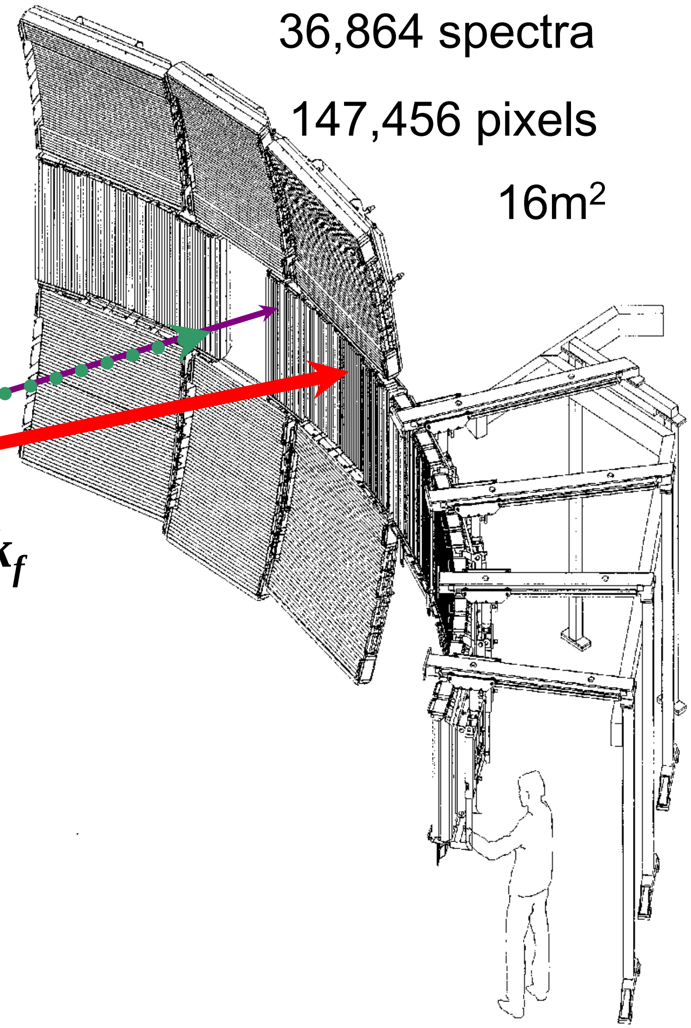
Merlin time-of-flight spectrometer
As time of flight is changed both energy transfer and wavevector transfer change for each detector

36,864 spectra

147,456 pixels

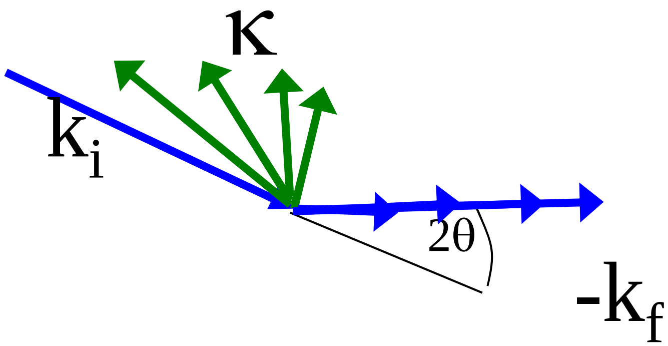
16m^2

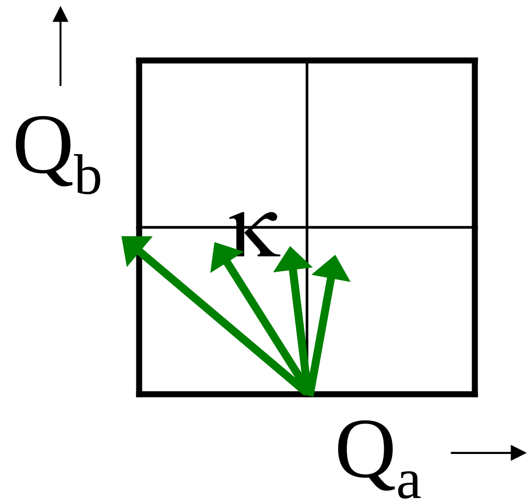




$$E = E_i - E_f = \frac{\hbar^2}{2m_n}\left(k_i - k_f^2\right) = \frac{1}{2}m_n\left(v_i^2 - v_f^2\right) = \frac{1}{2}m_n\left[\left(\frac{d_i}{t_i}\right)^2 - \left(\frac{d_f}{t_f}\right)^2\right]$$

Time of Flight Spectrometer – Measuring





- Every detector trances a different path in E and Q transfer
- A large dataset is obtained from all detectors containing intensity as a function of three dimensional wavevector and energy

Time of Flight Spectrometer – Pros and Cons

Advantages

- It is possible to simultaneously measure a large region of energy and wavevector space and get an overview of the excitations
- This allows unexpected phenomena to be observed
- It does not have the same problem of second order scattering as the triple axis spectrometer

Disadvantages

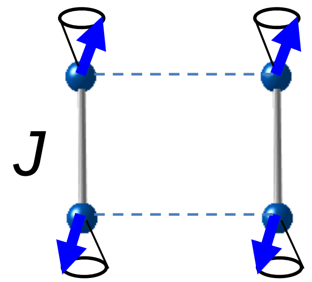
- Time-of-flight instrument have low neutron flux for an specific wavevector and energy but the ESS will be different
- It is difficult to do polarised neutron scattering

Example 1
Zero Dimensional
Quantum Magnets

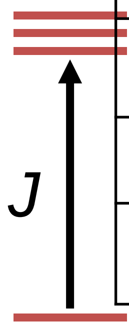
0-Dimensions - Spin-1/2, Dimer Antiferromagnets

Dimer Unit
S=1/2, $S^z=\pm 1/2$

$$\hat{H} = J\hat{S}^a \cdot \hat{S}^b$$

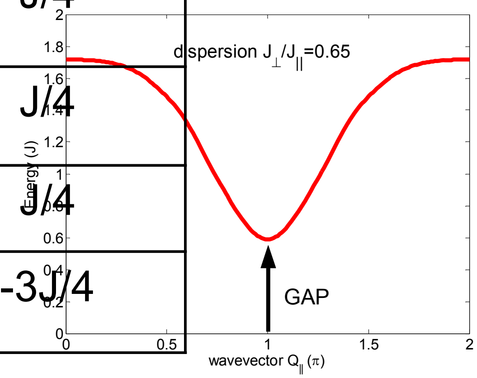


Excitations

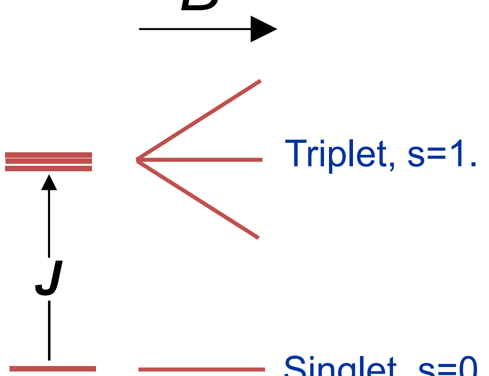


Eigenstates	S_T	S^z	Eigenvalue
$\vert +1\rangle = \vert\uparrow_1\uparrow_2\rangle$	1	1	J/4
$\vert 0\rangle = \frac{1}{\sqrt{2}}(\vert\uparrow_1\downarrow_2\rangle + \vert\downarrow_1\uparrow_2\rangle)$	1	0	J/4
$\vert -1\rangle = \vert\downarrow_1\downarrow_2\rangle$	1	-1	J/4
$\vert G\rangle = \frac{1}{\sqrt{2}}(\vert\uparrow_1\downarrow_2\rangle - \vert\downarrow_1\uparrow_2\rangle)$	0	0	-3J/4

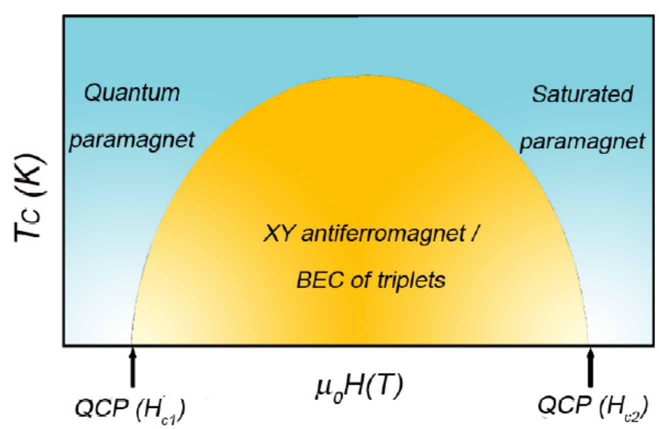
Interdimer coupling, gapped dispersive Mode



Zeeman Splitting in Field



Bose Einstein Condensation



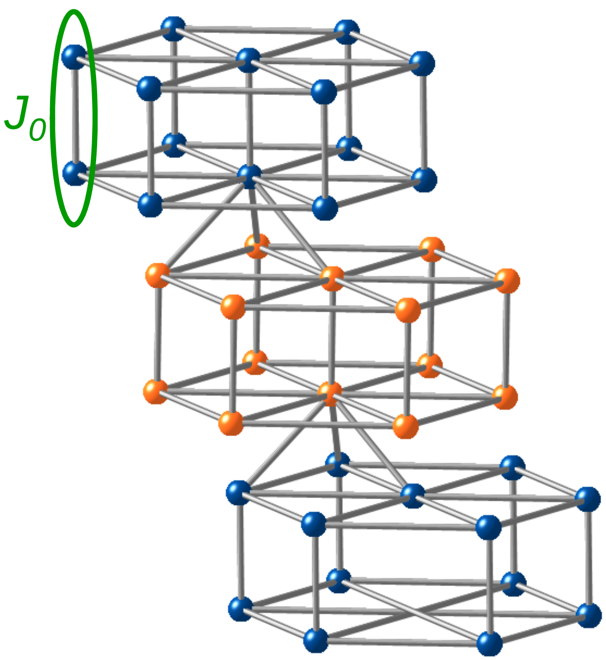
Properties:

- Singlet ground state.
- Gapped 1-magnon
- 2-magnon continuum
- Bound modes.
- Bose Einstein condensation.

$Sr_3Cr_2O_8$ –Spin-1/2, Dimer AF

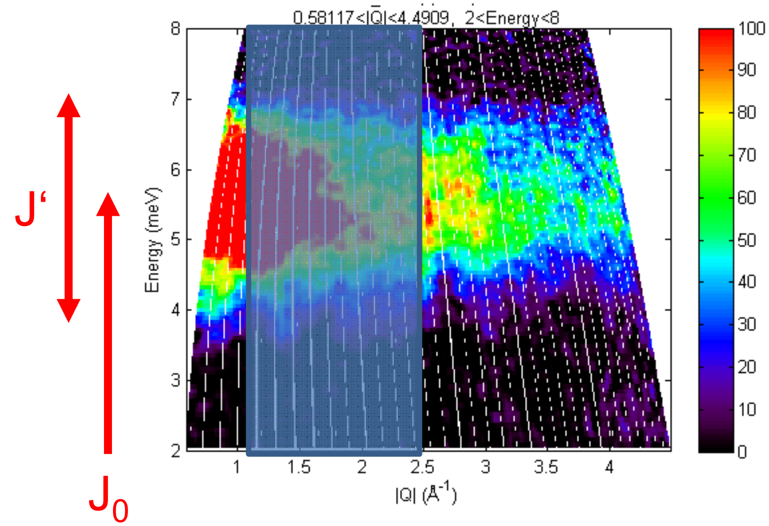
$Sr_3Cr_2O_8$ → Cr^{5+}, Spin-1/2.

Space group - R-3m

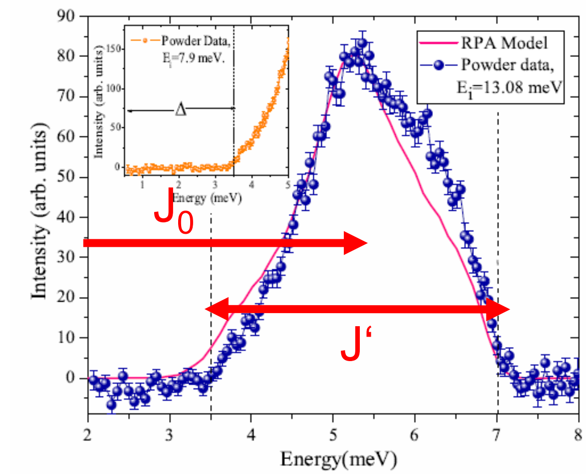


Powder inelastic neutron scattering

D.L. Quintero-Castro, et al Phy. Rev. B. 81, 014415 (2010)



E_{gap}=3.4meV
E_{upper}=7.10meV



Dimer coupling is bilayer J_0

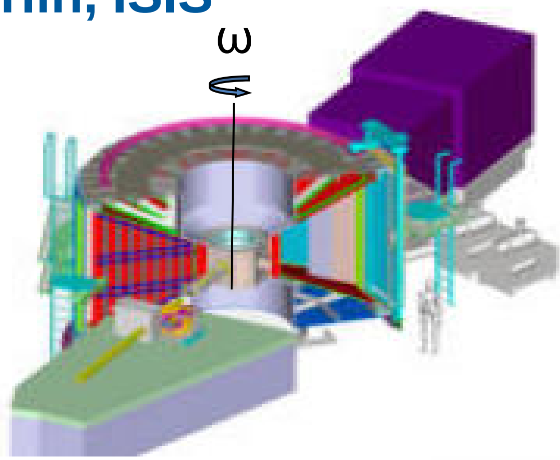
$E_{midband}$~J_0=5.5meV
$E_{bandwidth}$~J'=3.7meV

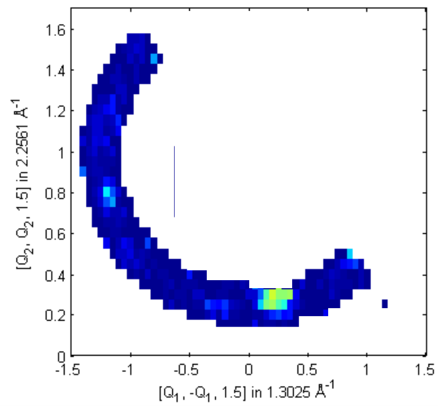
$Sr_3Cr_2O_8$ is 3D network of dimers

B. Lake; Tartu, Sept 2017

Single Crystal Inelastic Neutron Scattering

Merlin, ISIS



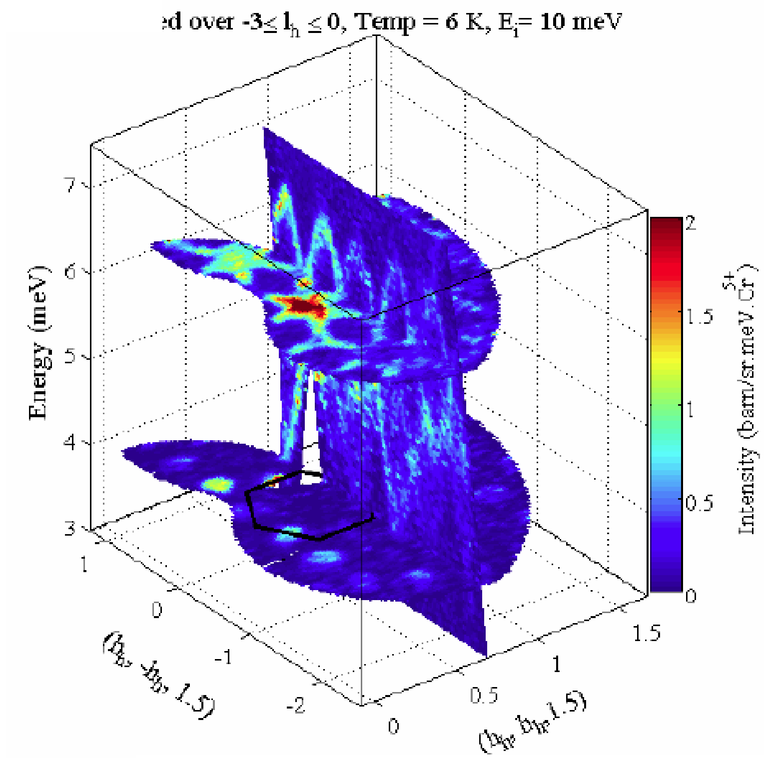


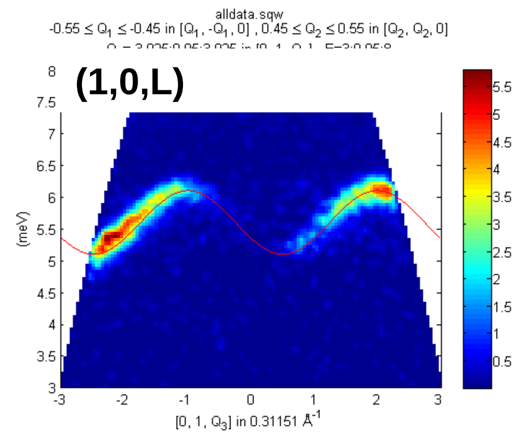
Individual scans combined to create a single file $S(Q_h, Q_k, Q_l, E)$.

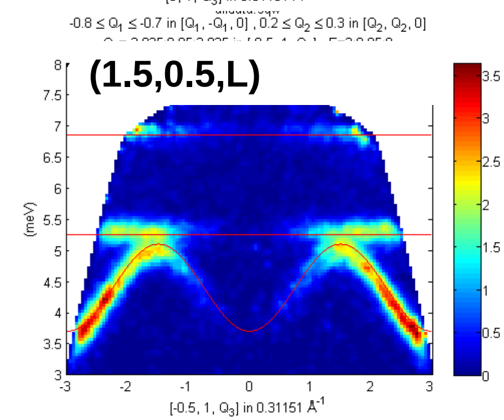
large region of the energy and reciprocal space.

detectors:
180° horizontal
±30° vertical

ω scans,
Range 70°
step=1°
2 hours per step.





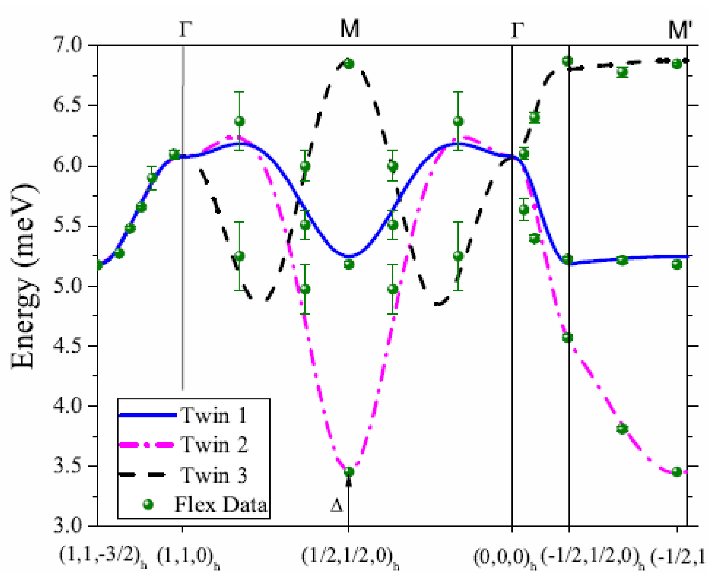


B. Lake; Tartu, Sept 2017

D.L. Quintero-Castro, et al Phy. Rev. B. 81, 014415 (2010)

Fitting to a Random Phase Approximation

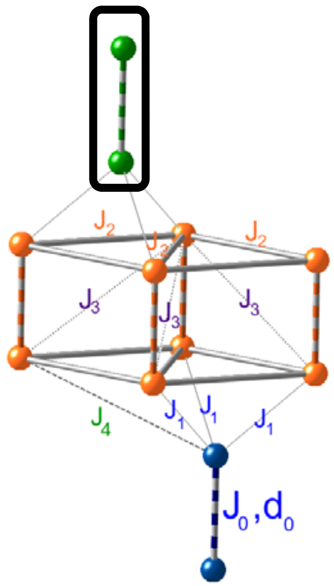
Extracted Dispersions



Random Phase Approximation

M. Kofu et al Phys. Rev. Lett. 102 037206 (2009)

$$\hbar\omega \cong \sqrt{J_0^2 + J_0\gamma(\mathbf{Q})} \qquad \gamma(\mathbf{Q}) = \sum_i J(\mathbf{R_i})e^{-i\mathbf{Q}\cdot\mathbf{R_i}}$$



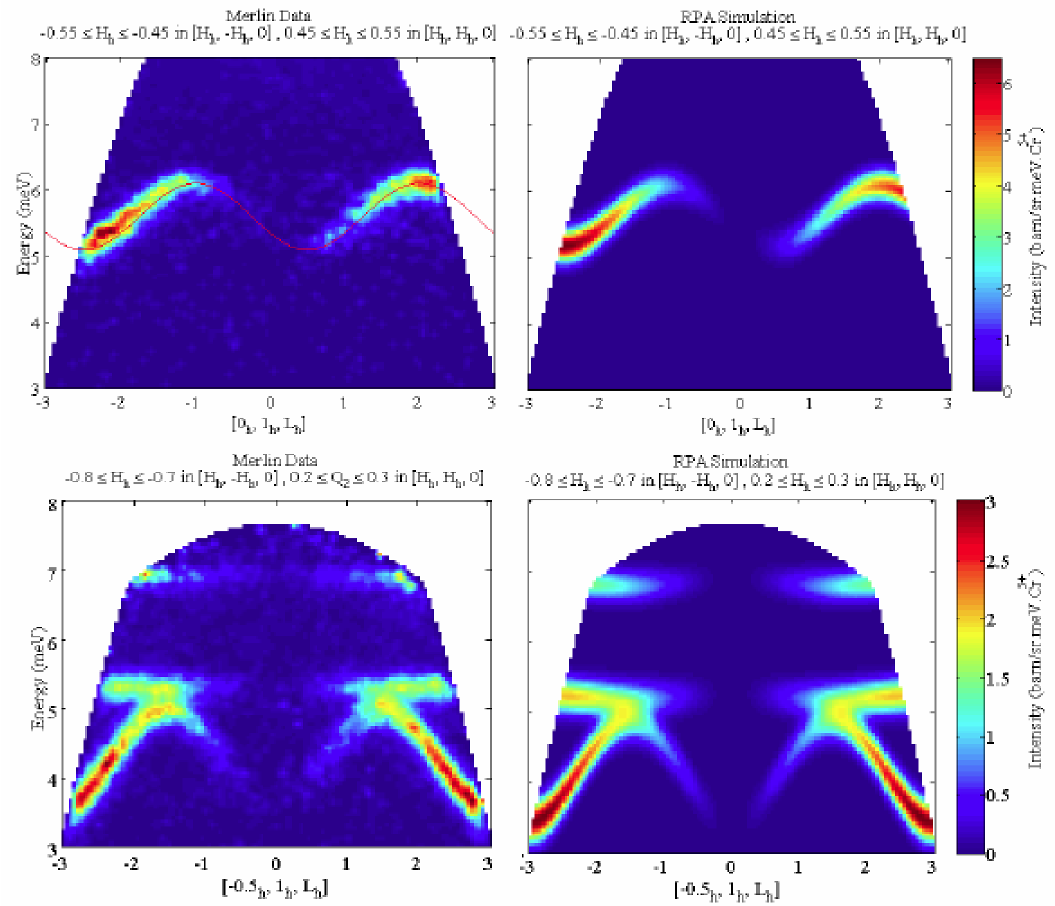
Constants	$Sr_3Cr_2O_8$
J_0	5.551(9)
J_1'	-0.04(1)
J_1''	0.24(1)
J_1'''	0.25(1)
$J_2' - J_3'$	0.751(9)
$J_2'' - J_3''$	-0.543(9)
$J_2''' - J_3'''$	-0.120(9)
J_4'	0.10(2)
J_4''	-0.05(1)
J_4'''	0.04(1)
$J' =$	$J' = 3.6(1)$
J'/J_0	$J'/J_0 = 0.6455$

Simulation and Data

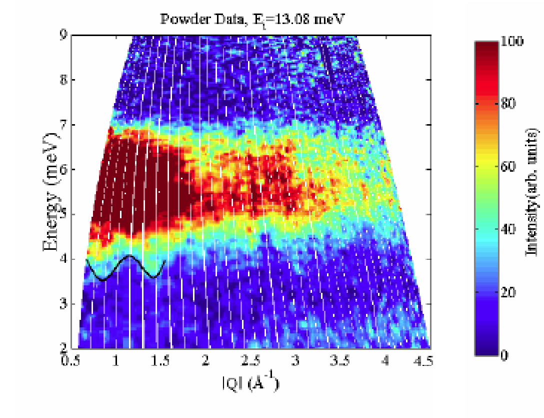
Neutron cross-section

$$\frac{d^2\sigma(\mathbf{Q},E)}{d\Omega dE} \approx \frac{\left|f_{Cr^{5+}}(|Q|)\right|^2 (1 - cos(\frac{2\pi \ell_h d_0}{c_h}))e^{(-(E-\hbar\omega)^2/\Delta E^2)}}{\hbar\omega(1 - e^{E/k_B T})}$$

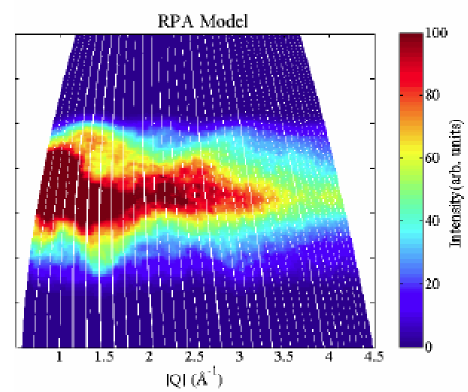
Data – single crystal   simulation – single crystal



Data - Powder average:



Simulation - Powder average:

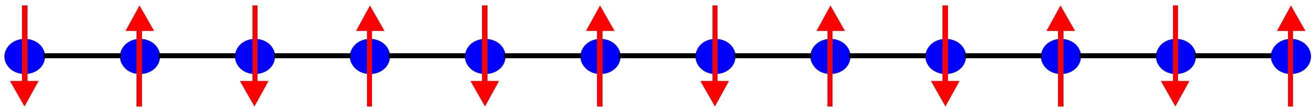


D. L. Quintero-Castro, B. Lake, E.M. Wheeler
Phy. Rev. B. 81, 014415 (2010)

Simulation of the TOF data with the fitted values interactions

Example 2
One Dimensional Quantum Magnets

1D, S-½, Heisenberg, Antiferromagnet



$$H = J\sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

Bethe Ansatz

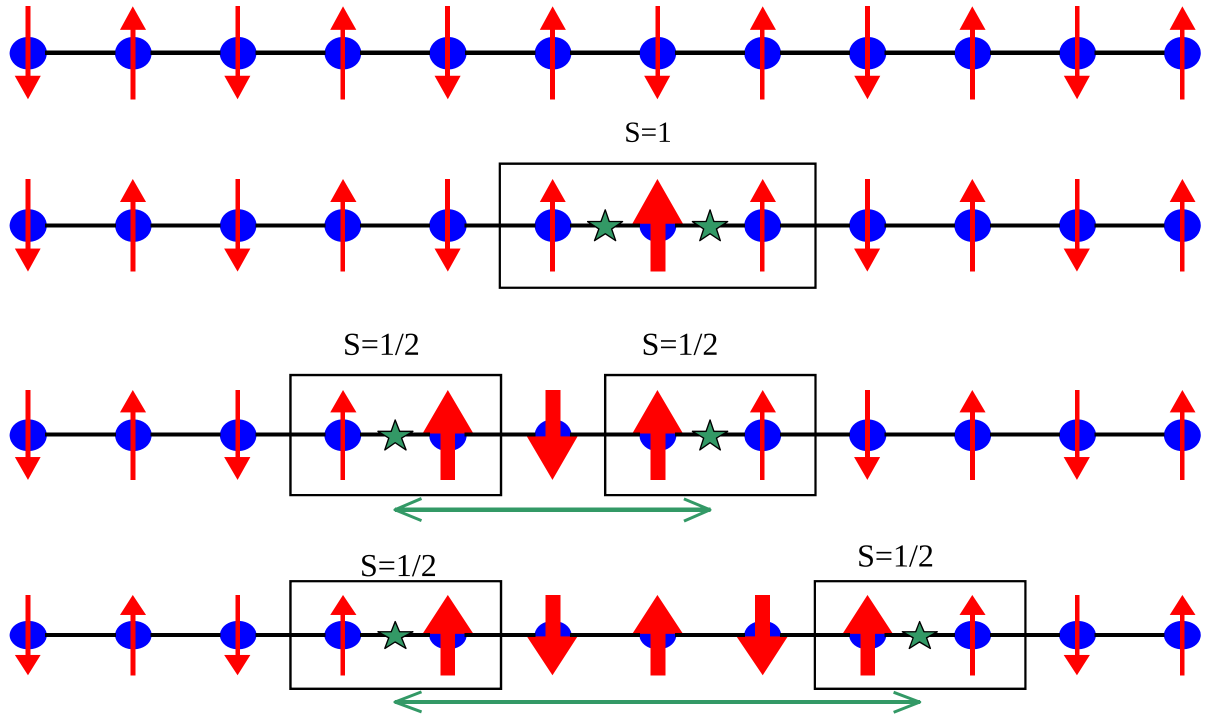
Hans Bethe
Bethe Ansatz
(1931)

- Ground state has no long-range Néel order.
- Ground state consists of 50% spin-flip states
- All combinations must be considered.
- Little physical insight into the quasi-particles.

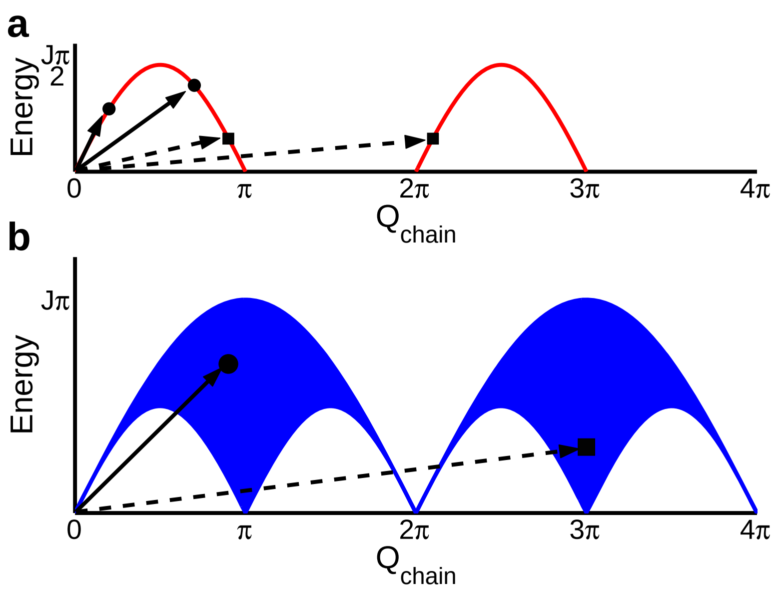
The Bethe Ansatz has been a long standing problem of theoretical condensed matter

Spinons Excitations

Fadeev and Taktajan (1981)



The fundamental excitations are spinons not magnons.



Spinons
- Fractional spin-½ particles
- created in pairs
- spinon-pair continuum

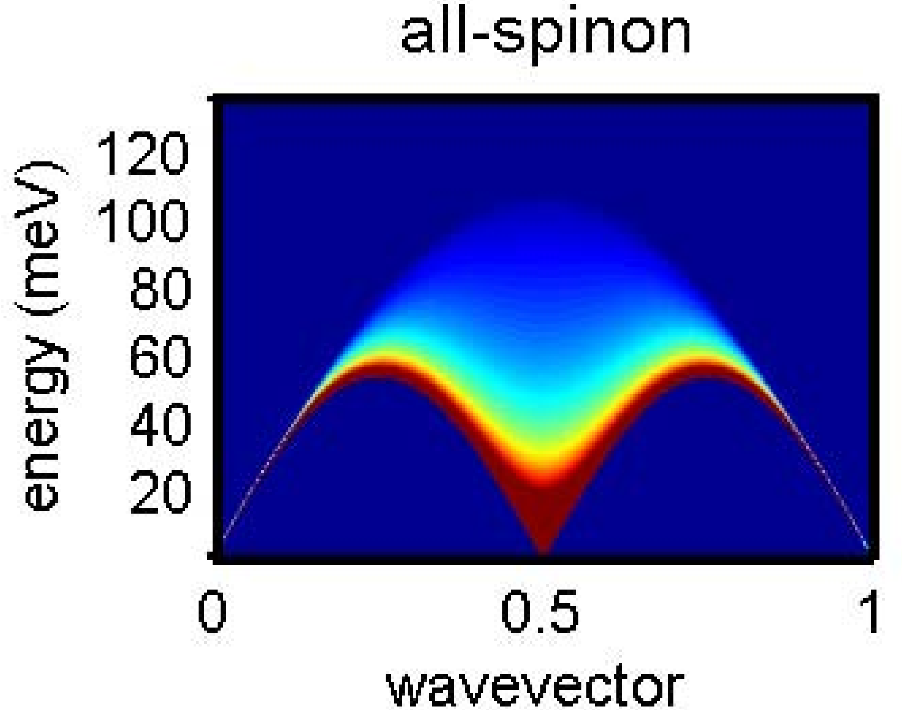
Solution of Bethe Ansatz

Several approximate theories have since been postulated for the spinon continuum of the spin-1/2 Heisenberg chain

- Müller Ansatz
- Luttinger Liquid Quantum Critical point

In 2006 J.-S. Caux and J.-M. Maillet solved the 1D, spin-1/2, Heisenberg, antiferromagnet, 75 years after the Bethe Ansatz was proposed.

J.-S. Caux,
R. Hagemans,
J. M. Maillet
(2006)



1D S-1/2 Heisenberg Antiferromagnetic - $KCuF_3$

Cu^{2+} ions S=1/2

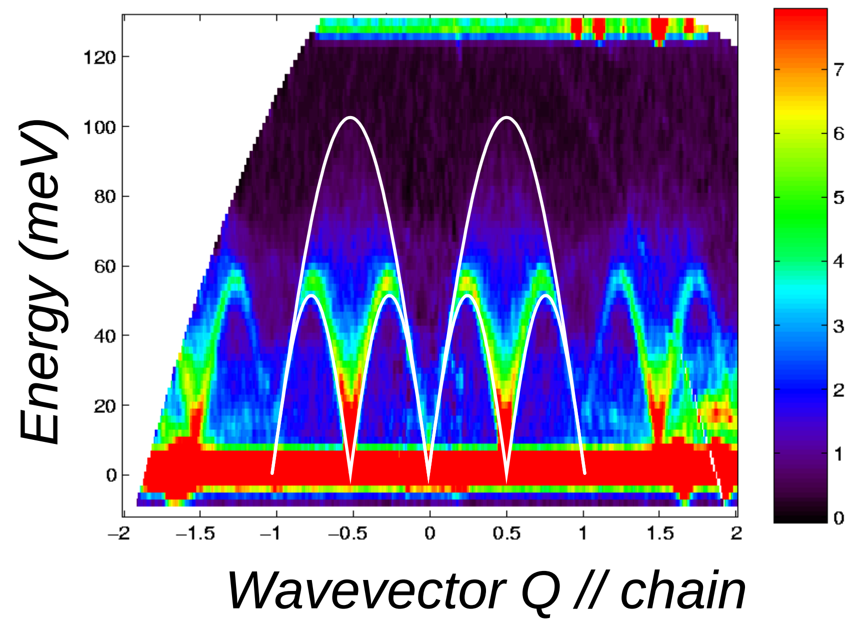
Antiferromagnetic chains, $J_{//}$= -34 meV

Weak interchain coupling, $J_{\perp}/J_{//}$ ~ 0.02

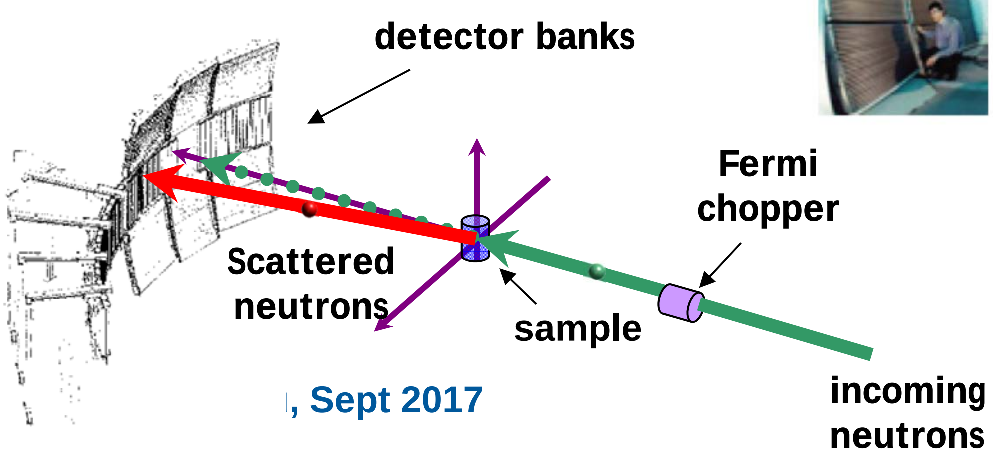
Antiferromagnetic order T_N ~ 39K

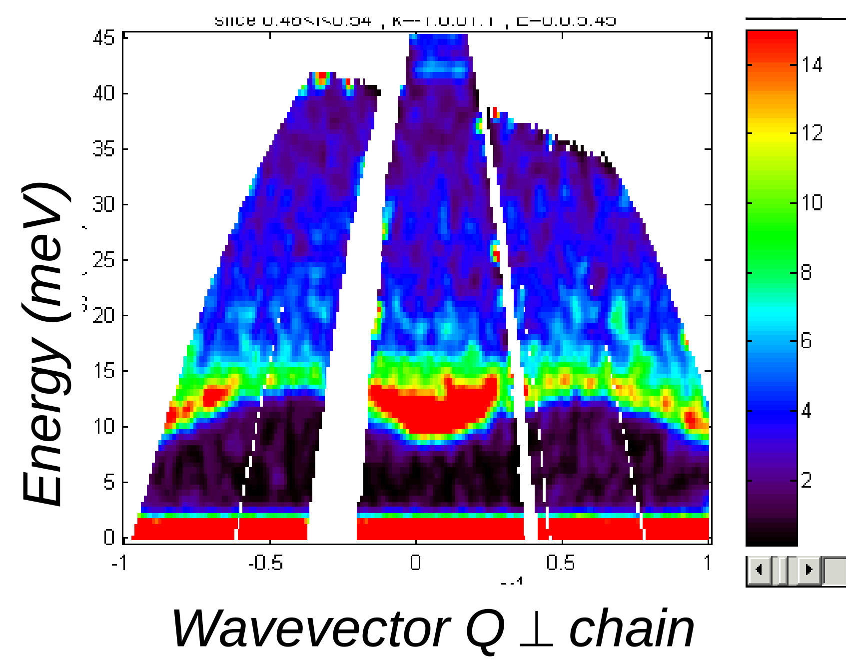
Only 50% of each spin is ordered

$$\hat{H} = J_{\parallel}\sum_{r}\vec{S}_{r,l}\cdot\vec{S}_{r+1,l} + J_{\perp}\sum_{l,\delta}\vec{S}_{r,l}\cdot\vec{S}_{r,l+\delta}$$



MAPS neutron spectrometer, ISIS

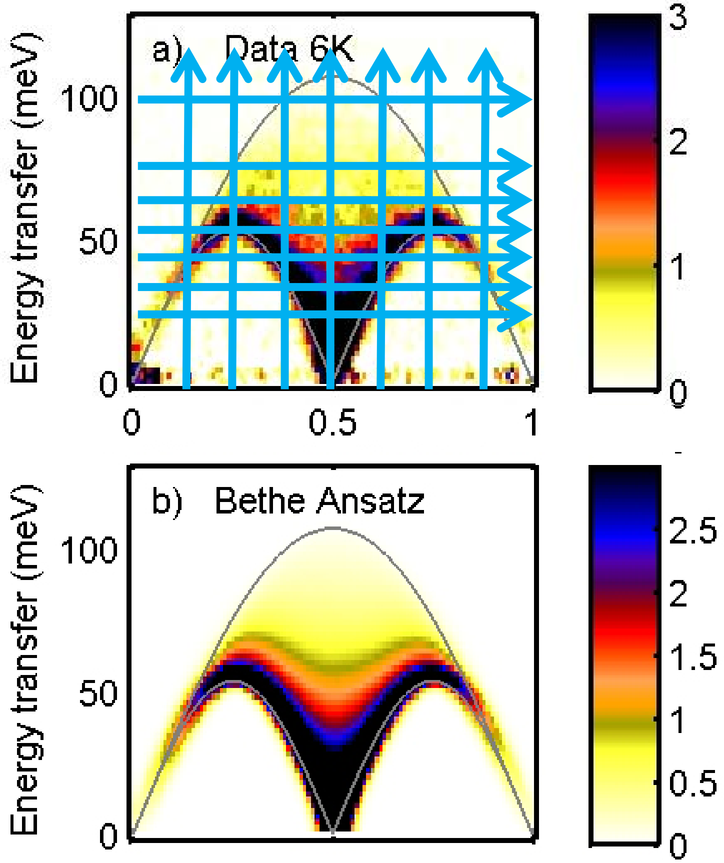


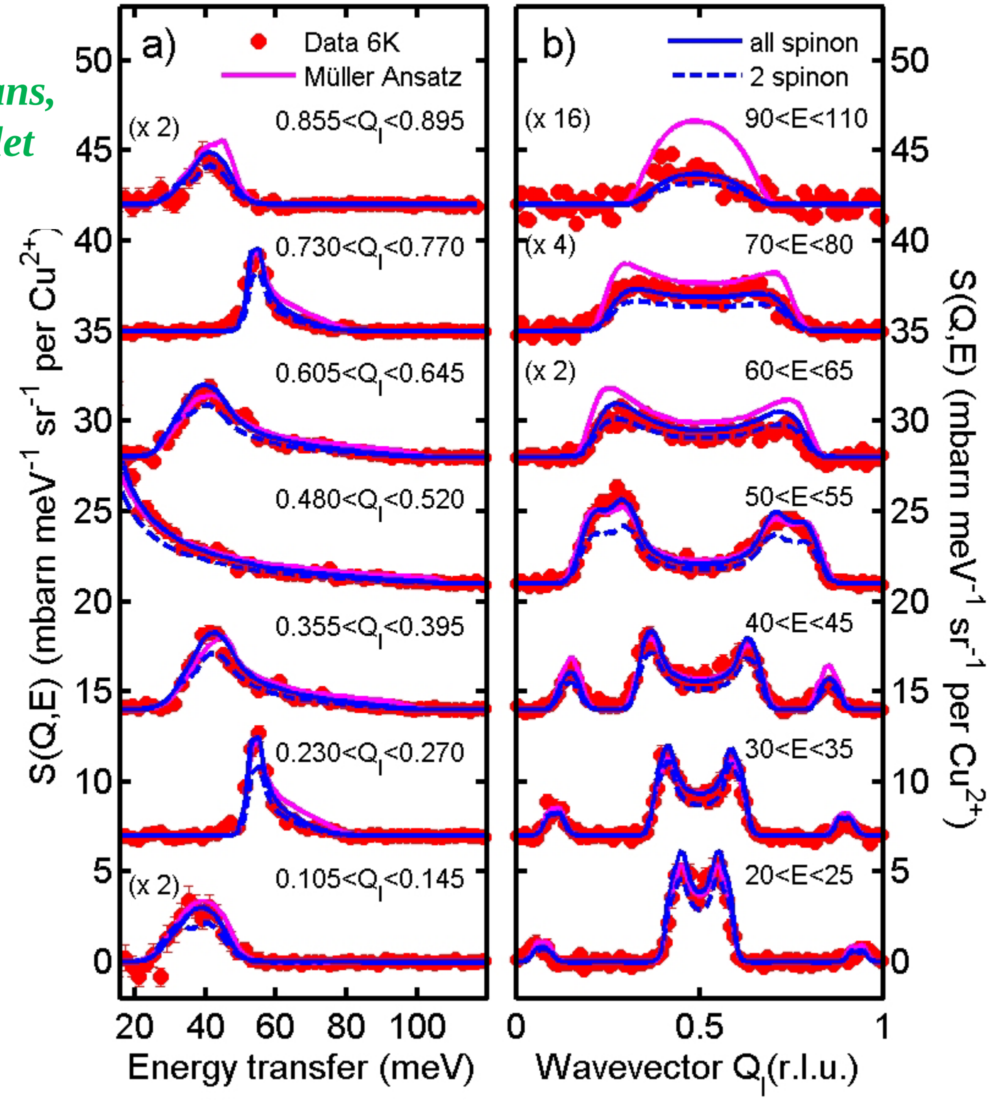


$KCuF_3$ compared to Bethe Ansatz, 2 and 4 spinons

Constant energy and constant-wavevector cuts compared to simulations

J.-S. Caux, R. Hagemans, J. M. Maillet (2006)



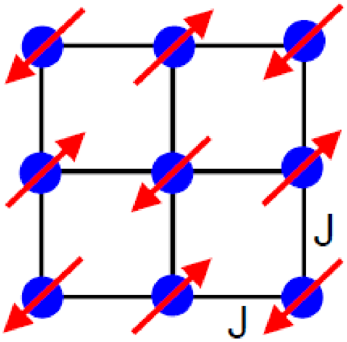


B. Lake et al, Phys. Rev. Lett. (2013)

B. Lake; Tartu, Sept 2017

Example 3
Two Dimensional
Quantum Magnets

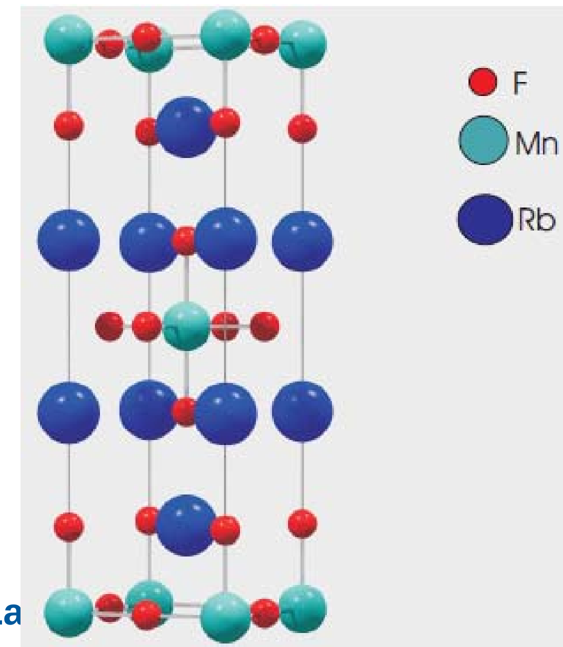
2-Dimensional Antiferromagnet - Square Lattice



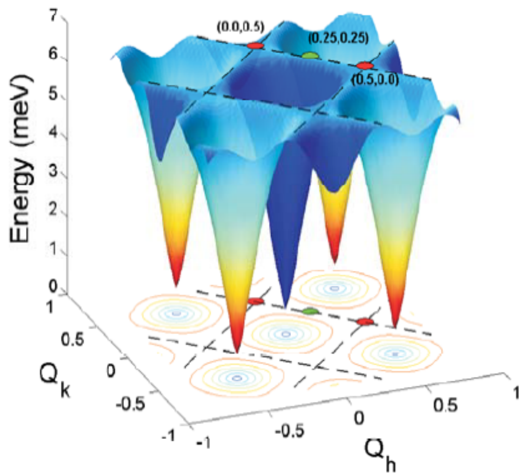
Ground state
long range order

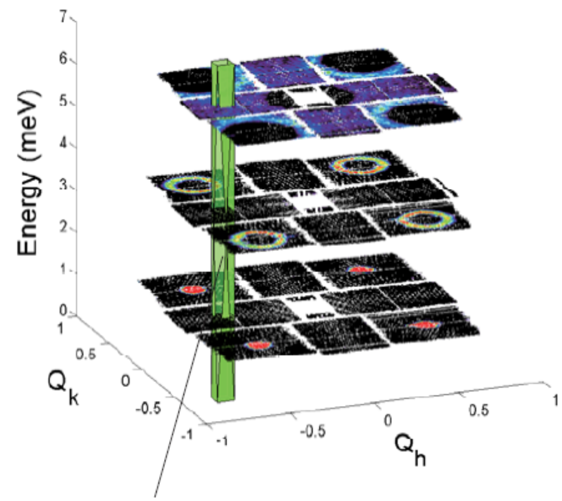
Excitations
Spin-waves

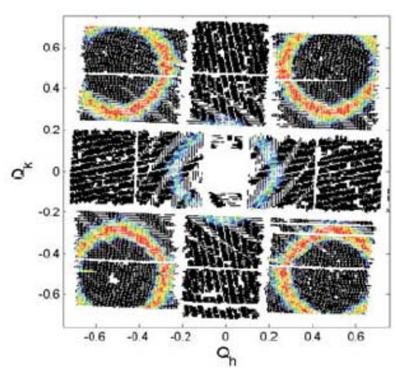
Rb_2MnF_4
2-Dimensional Spin-5/2
Heisenberg Antiferromagnet

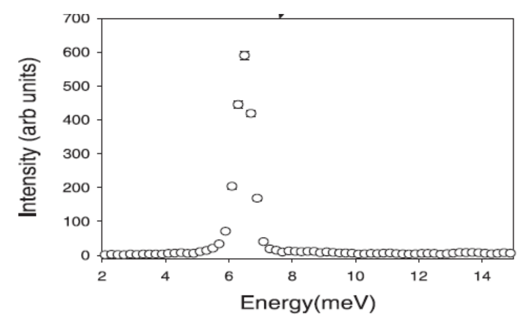


T Huberman et al J. Stat. Mech. (2008) P05017







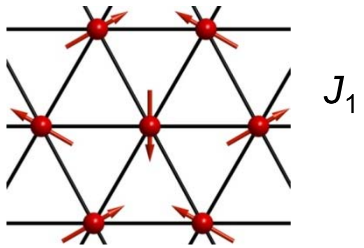


B. La

2-Dimensional Antiferromagnet - Triangular Lattice

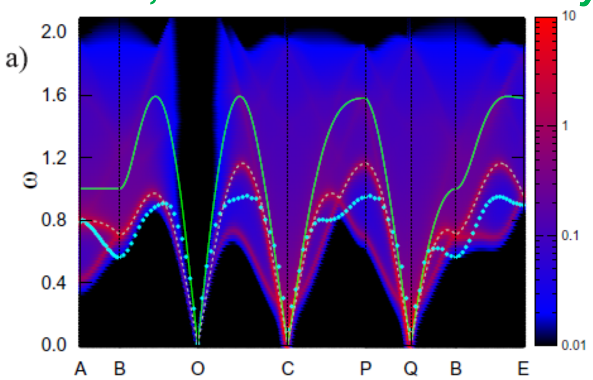
Triangular Lattice
Ground state – long range order

isotropic



$\varphi = 120°;\ \boldsymbol{k}_m = 1/3$

Excitations
A Mezio, et al New Journal of Physics (2012)

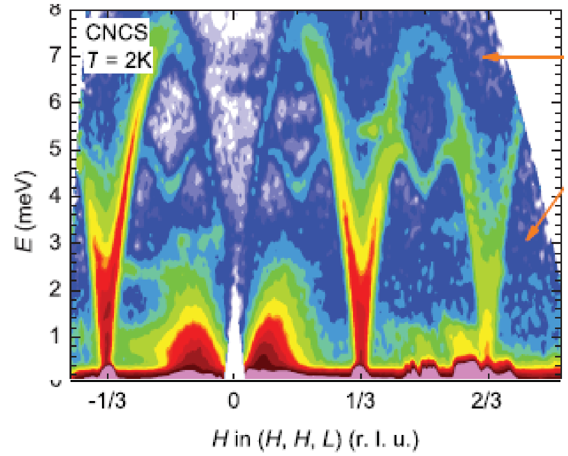


renormalised and broadened
compared to spin-wave theory

B. Lake; Tartu, Sept 2017

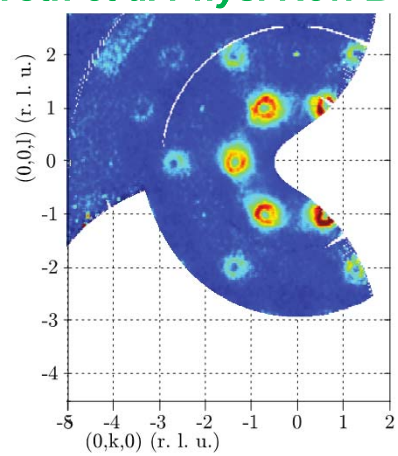
$CuCrO_2$ S-3/2, triangular lattice

M Frontzek et al Phys. Rev. B (2011)



Alpha-Ca_2CrO_4 S-3/2, triangular lattice

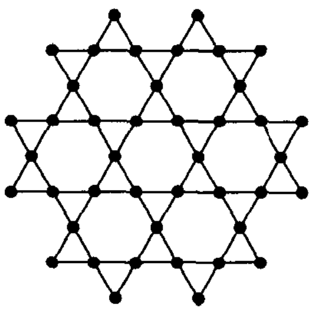
S Toth et al Phys. Rev. B (2011)

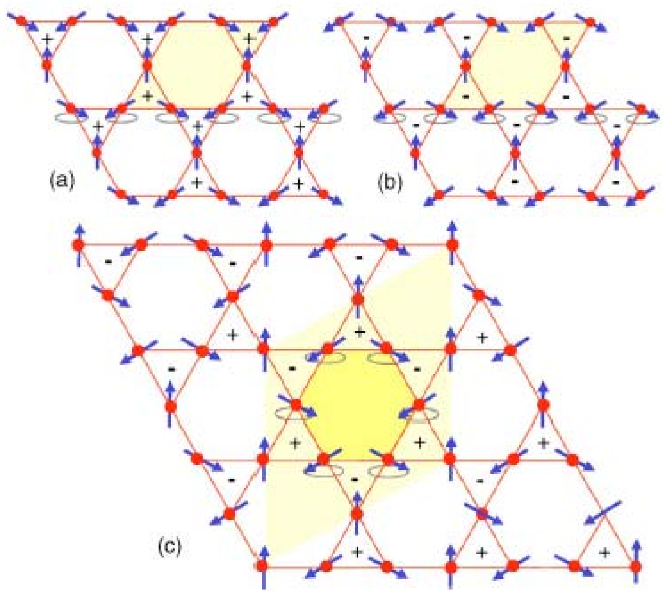


Ideal S-1/2, triangular antiferromagnet, $Ba_3CoSb_2O_9$ H. Tanaka et al

2-Dimensional Antiferromagnet - Kagome Lattice

Kagome Lattice

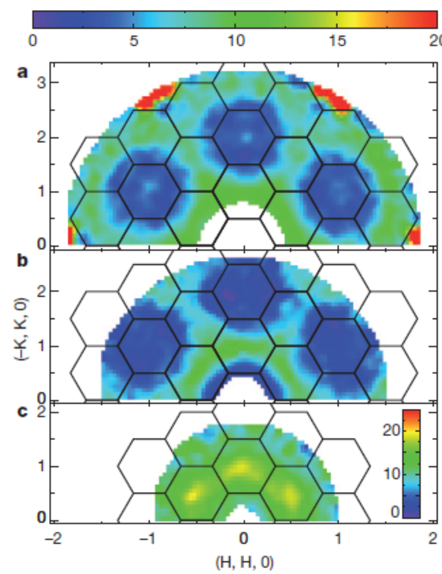


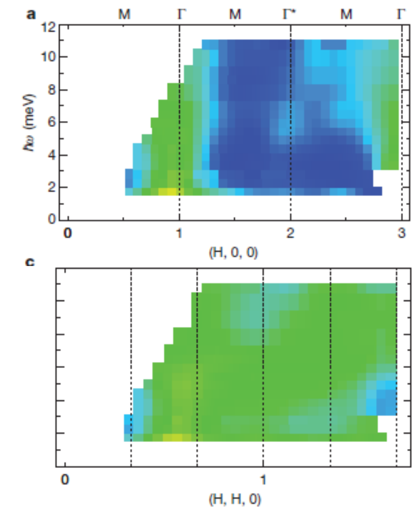


S-5/2
Long-range order
Spin-wave excitation

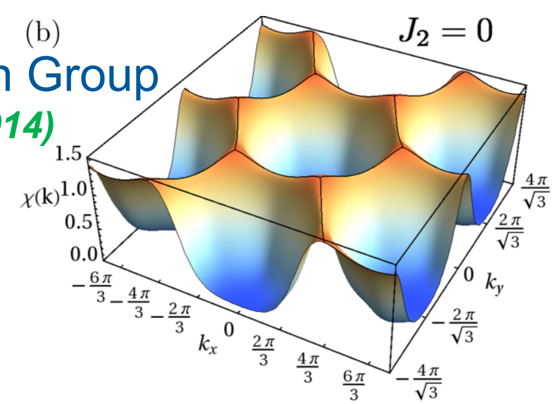
S-1/2
no order
diffuse excitations

e.g. Herbertsmithite
T.-H. Han
Nature 492, 406 (2012)



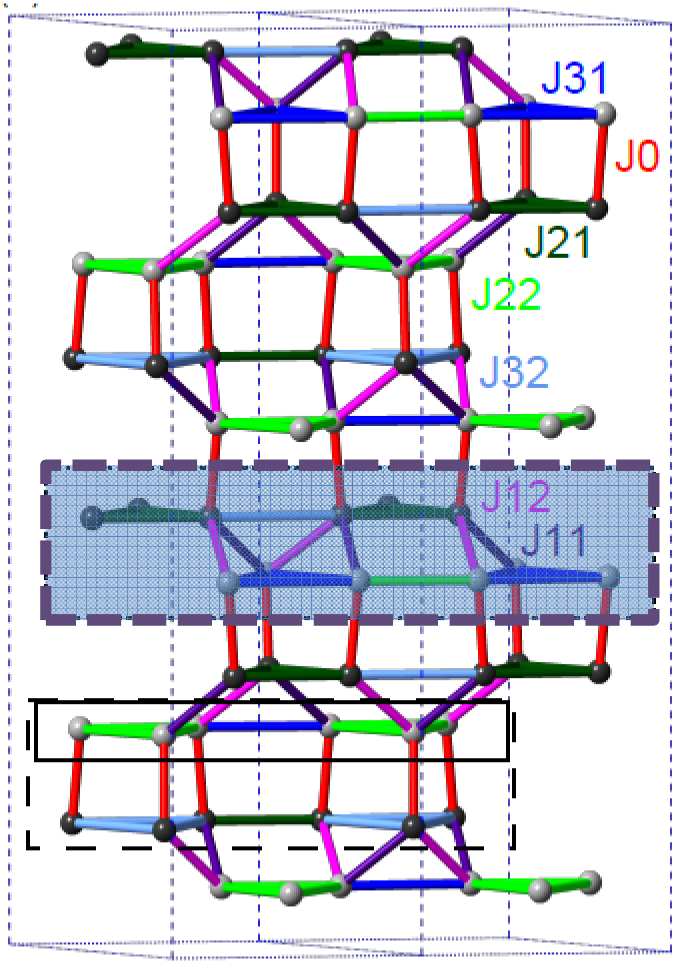


Pseudo-Fermion
Functional Renormalisation Group
R. Suttner, et al Phys. Rev. B (2014)



B. L

$Ca_{10}Cr_7O_{28}$ - Crystal structure



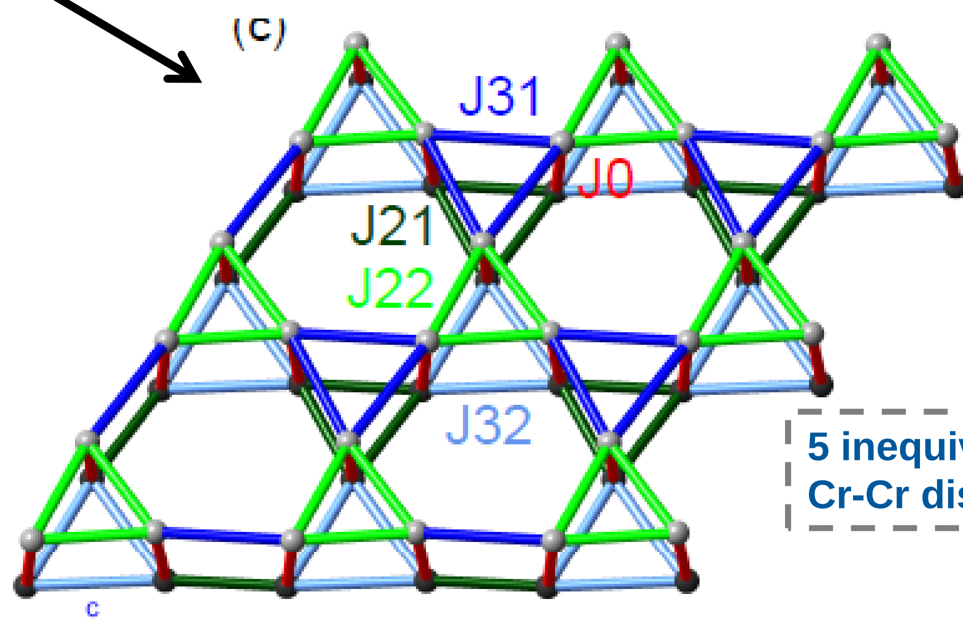
space group ***R3c***

D. Gyepesova, Acta Cryst. C69, 111 (2013)

- Cr^{5+} spin = ½ ions (1 electron in 3d-shell)
- 7 different exchange path in structure
- No long-range magnetic order

Kagome bilayer model

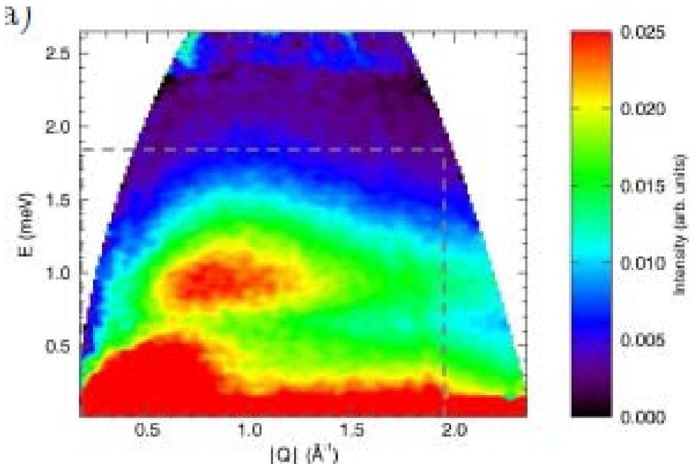
- *a-b* plane shows distorted kagome bilayers
- large blue and small green triangles alternate within each layer, and between layers



5 inequivalent Cr-Cr distances

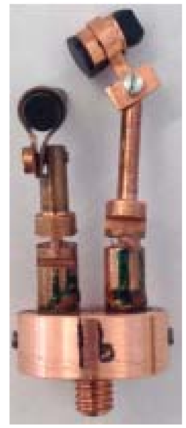
Inelastic Neutron Scattering – Zero Field

Powder; TOFTOF, FRM2; T=0.43K

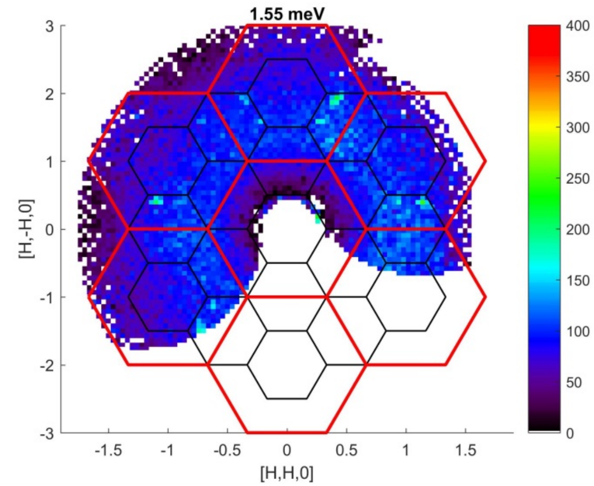


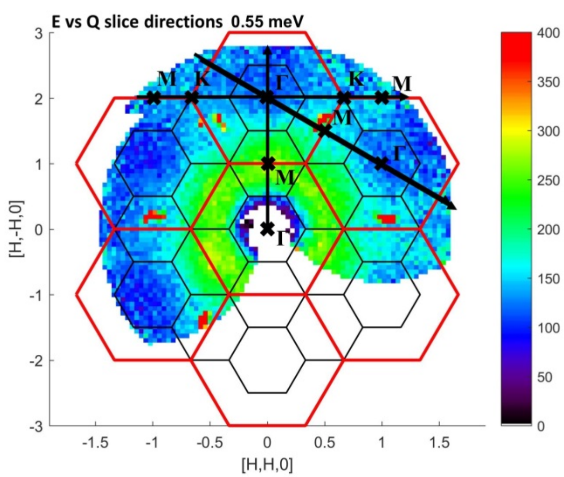
- Excitations to 1.6meV
- Two Bands of excitations

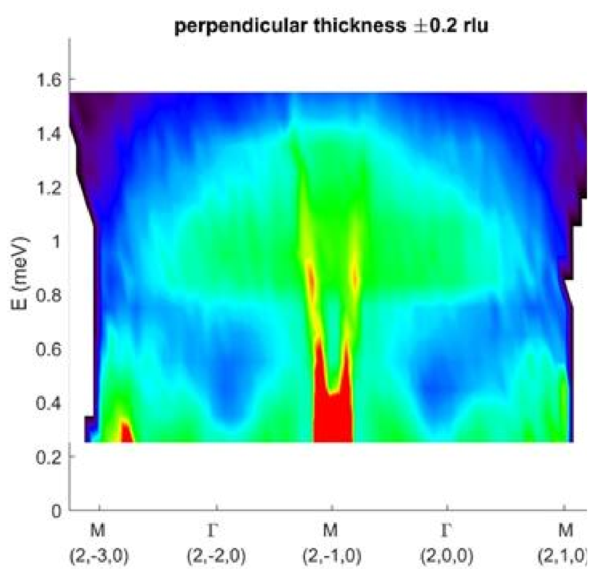
Single Crystals

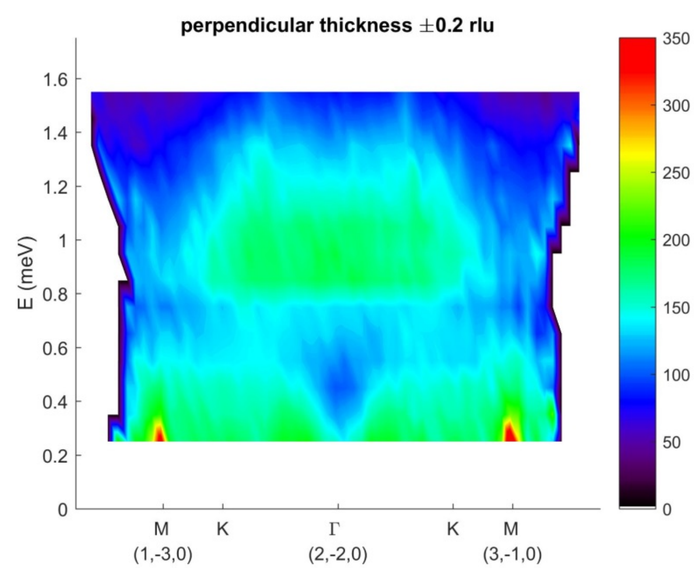


[H,K,0]; MACS, T=0.09K









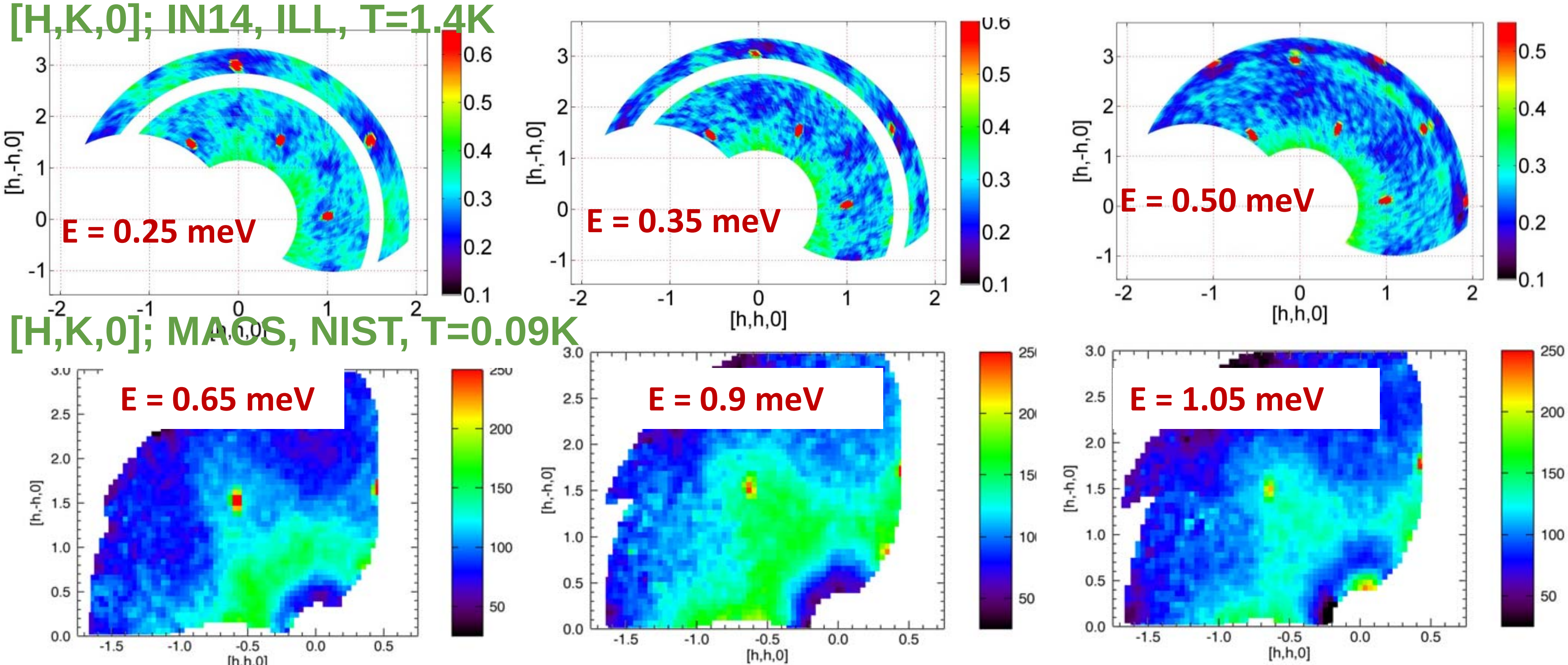
C. Balz, B.Lake, J. Reuther et al Nature Phys. 12, 942 (2016)

Broad diffuse scattering

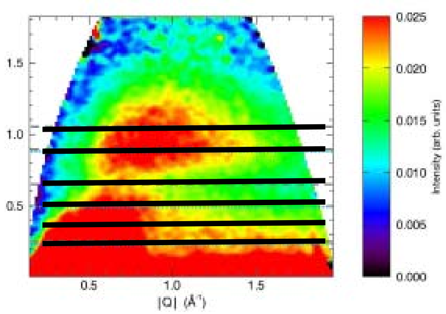
Inelastic neutron scattering – Zero field, single crystal

[H,K,0]; IN14, ILL, T=1.4K

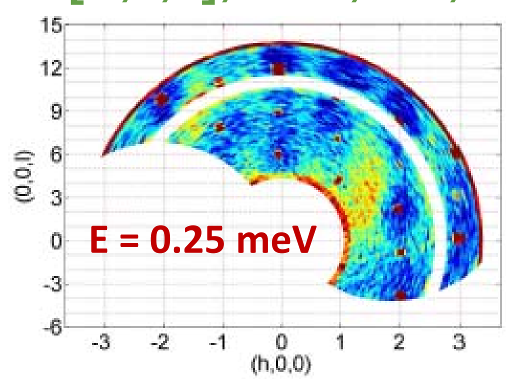
[H,K,0]; MACS, NIST, T=0.09K



Powder
T=0.43K



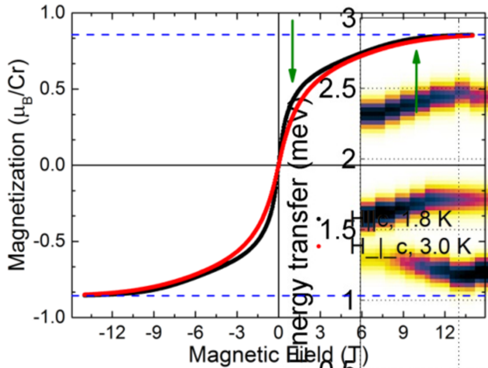
[H,0,L]; IN14, ILL, T=1.4K

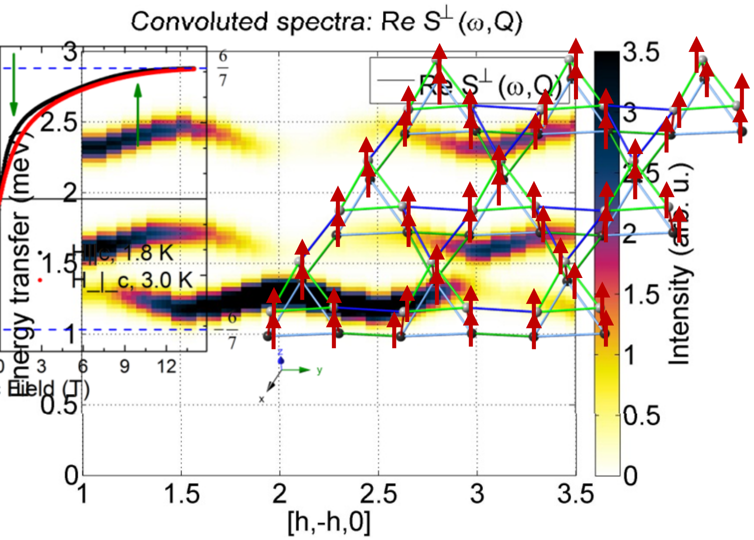


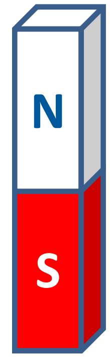
- Quasi 2D correlations
- Broad Diffuse Scattering **no spin-waves, spinons?**

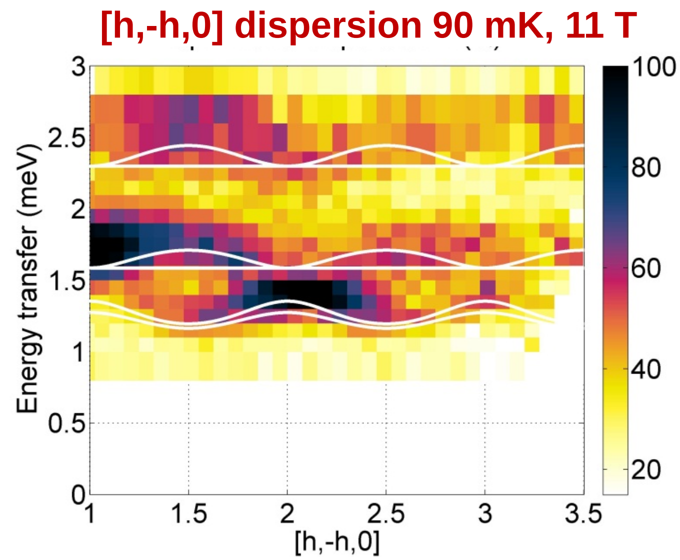
$Ca_{10}Cr_7O_{28}$ - Inelastic neutron scattering – High-field

Ferromagnetic order at H=11T ⇒ spin-waves

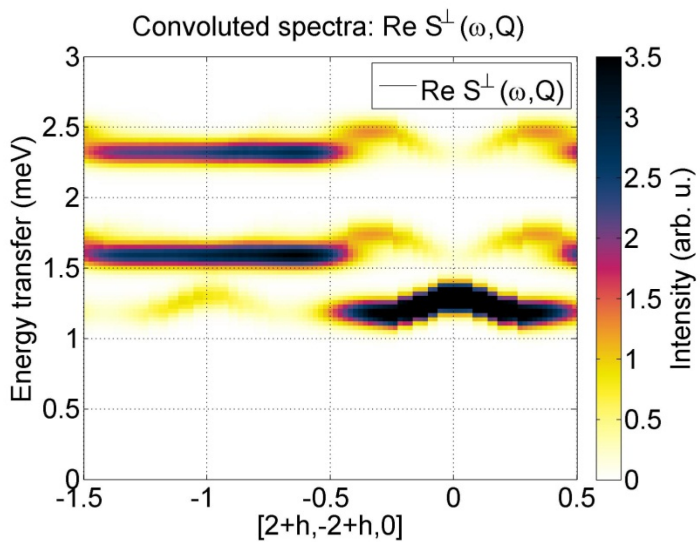


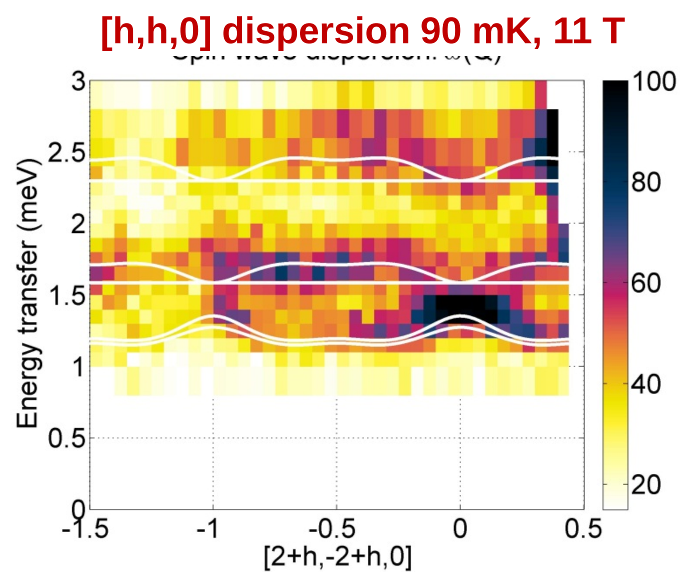






- Sp
- Sp





B. Lake; Tartu, Sept 2017

C. Balz, B. Lake, J. Reuther, Nature Physics 12, 942–949 (2016)

$Ca_{10}Cr_7O_{28}$ - Magnetic model - Exchange couplings

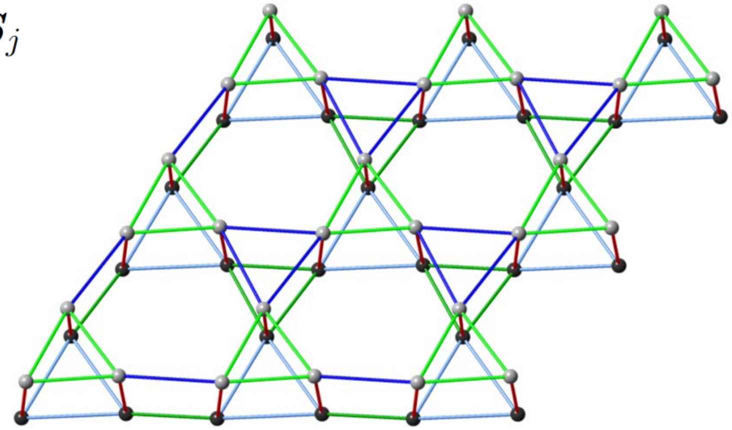
Exchange	Cr-Cr distance	Coupling constant	Type
	d [Å]	J [meV]	
J0	3.883	-0.0794	FM
J21	5.033	-0.7615	FM
J22	5.095	-0.2696	FM
J31	5.697	0.0876	AFM
J32	5.750	0.1072	AFM
ΣJ		-0.9158	

$$\mathcal{H} = J_{ij} \sum_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

} FM intrabilayer

} FM triangles

} AFM triangles

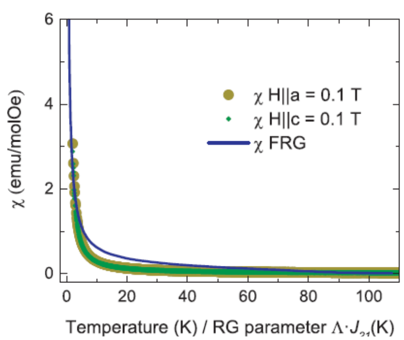


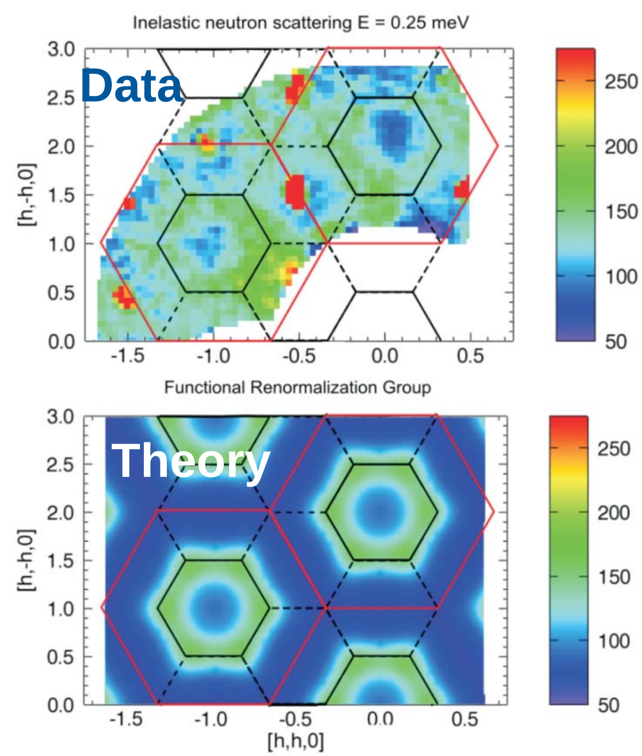
Pseudo-Fermion Functional Renormalisation Group

Using the Hamiltonian extracted from INS

⇒ Susceptibility shows no long-range order

⇒ Diffuse magnetic scattering



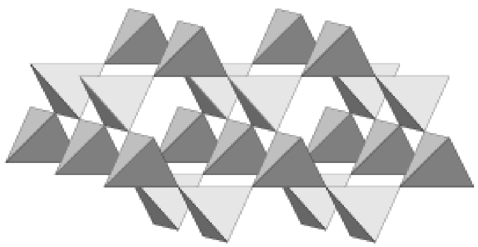


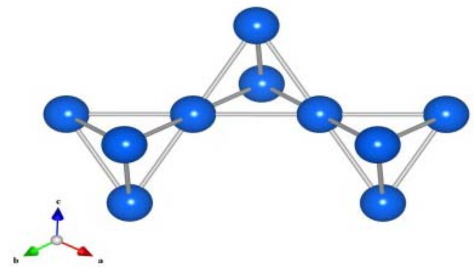
Non-ordered ground state, diffuse spinon scattering.
Reveals highly robust spin liquid state

Example 4
Three Dimensional
Quantum Magnets

Frustrated 3-Dimensions Magnets – Pyrochlore Lattice

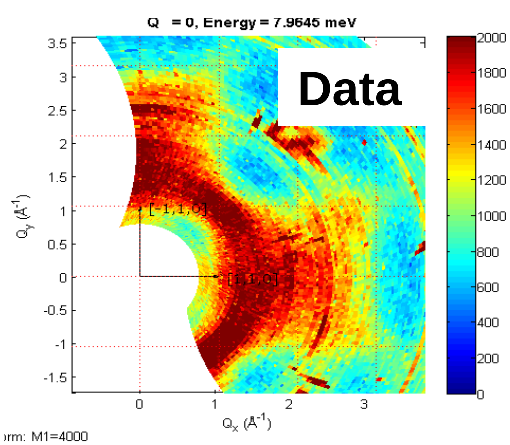
Pyrochlore Lattice – corner-sharing tetrahedra

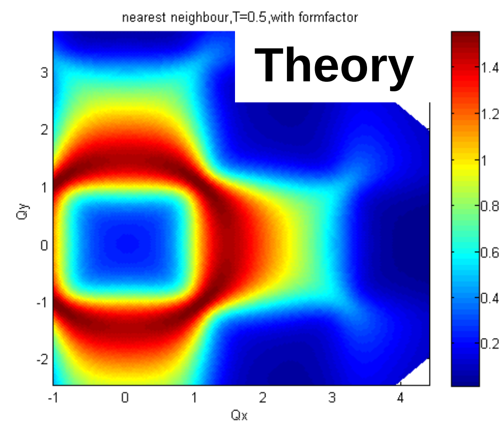




Interconnected chains
Antiferromagnetic J
3D frustration

MgV_2O_4, V has spin-1



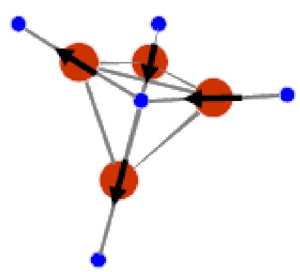


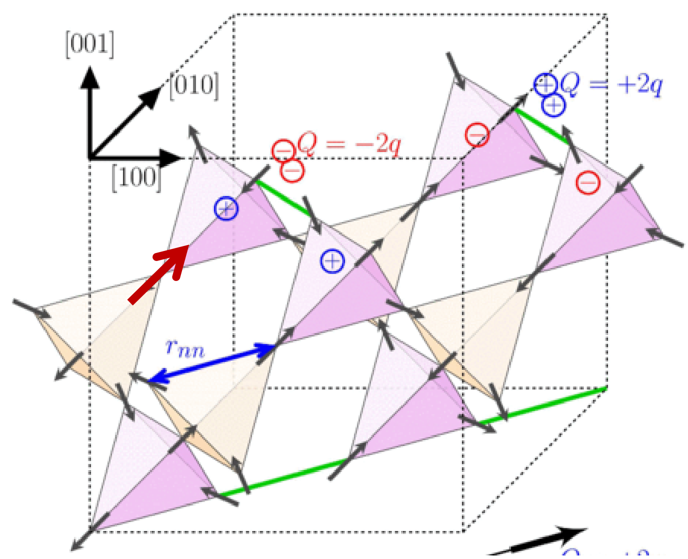
Constant Energy E=8meV, IN20 with Flatcone
reveals broad diffuse scattering very different from spin-wave excitations

B. Lake; Tar

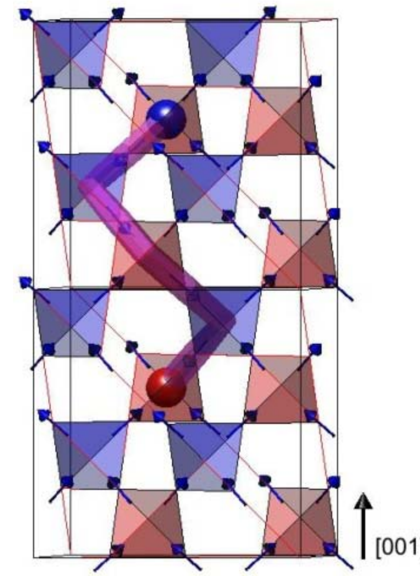
3-Dimensions - Pyrochlore Magnets

Spin Ice
- Ferromagnetic interactions
- Strong Ising anisotropy
- Ice rules 2 in, 2 out

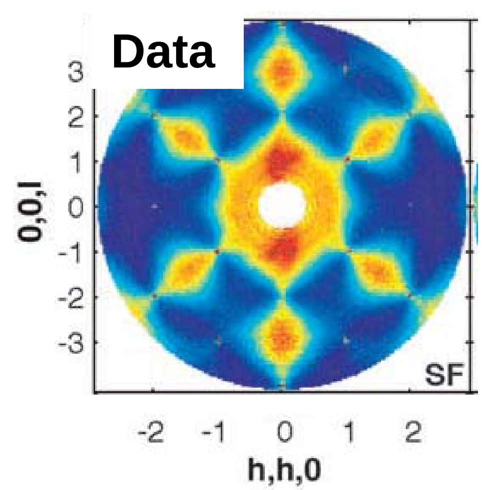


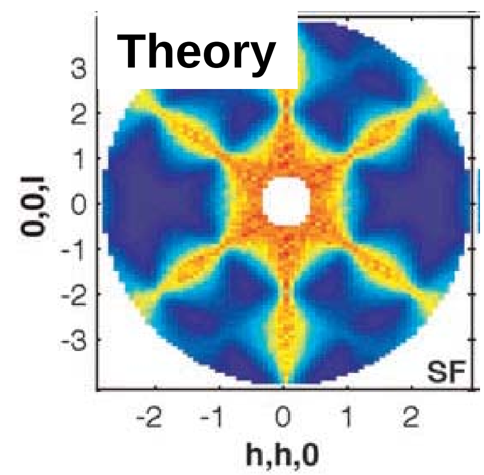


Ground state - topological order



Excitations - monopoles





T. Fennell et al Science 326 415 (2009)
D.J.P. Morris, et al Science 326, 411 (2009)

Summary

Conventional Magnets

Long-range magnetic order and spin-wave excitations

Origins of Quantum magnetism

low spin values, antiferromagnetic, low-dimensional, frustration, spin liquids

Neutron scattering for quantum magnets

Inelastic neutron scattering

Triple Axis spectrometer, time-of-flight spectrometer

Examples of frustrated magnets

0-dimensional magnets e.g. dimer magnets

1.Dimensional magnets e.g. the spin-1/2 chain

2-Dimensional magnets e.g. Square, triangular, kagome, lattice

3-Dimensional magnets e.g. pyrochlore, spin ice and water ice

Beyond long-range magnetic order and spin-wave theory there are many unusual quantum states to be explored