Magnetic Neutron Scattering

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I believe my talk is the only about magnetic properties of matter and therefore this slide gives a quick overview about the different orders of magnitude and corresponding methods of investigation of magnetic properties. With neutrons, the topic of this talk, we usually probe magnetism on an atomic scale. However, recent experiments show, that magnetic domains can successfully be studied by small angle scattering techniques. This method might be in future of importance for the study of antiferromagnetic domains, which are not easy to study by any other method.
Bragg’s Law in Reciprocal Space (Ewald Sphere)

\[ |Q| = 2 \sin(\Theta)|k| \]
Many other talks cover the principle of single crystal diffraction. In this example, the flat cone diffractometer E2, it is demonstrated, how a plane in reciprocal space can be mapped by neutron diffraction by rotating the sample and recording the scattered intensity on a position sensitive detector. Neutrons penetrate (usually) the sample and allow a rotation of 360 degrees.
The next transparencies give an overview on the calculation of the neutron scattering cross section. The formalism which has been developed is beautiful and covers a lot of different cases and therefore I present in detail. On this slide the definitions of the different types of cross sections are given. These can be measured by well calibrated instruments and compared to the results of theoretical model calculations. Let me emphasize, that in order to facilitate such a comparison, neutron instrumentation and theoretical modelling should be done on an absolute scale, i.e. in units of barn. It is a common practice, that experimental data is not well calibrated (in intensity) and theoretical models predictions are done in arbitrary units. To see how common this practice is, please just take the conference booklet and look at the plots in different talks, you will frequently find “arbitrary units” … I believe, that with relatively small effort scattering data can be put on an absolute scale and in this way it will be of much more use. I met several cases, where people were looking for an excitation in there data and discussed tiny peaks as probably crystal field levels – however, an inspection on an absolute intensity scale shows immediately, that the crystal field peaks should have a factor of 100 more intensity. We should try to avoid such an obvious misinterpretation of experimental data.

Another caveat which comes to my mind in this context is the frequent practice to recalculate the x-axis (energy, scattering angle) in a plot without proper transformation of the intensity: I use now the symbol “I” for the differential cross section - if I(Ω) is measured as a function of scattering angle Ω, it has to be plotted as I(Ω) vs Ω. If Ω is to be transformed to the scattering vector Q, then the proper transformation has to conserve the intensity, i.e. I(Ω)dΩ=I(Q)dQ. Therefore I(Q)=I(Ω) dQ/dΩ. Very frequently the factor dQ/dΩ is ignored, we should avoid such bad practice!

Let me start now with the theoretical evaluation of the double differential cross section, which is the most detailed quantity which can be studied without polarisation analysis of the neutrons (for polarized neutrons we would have to consider in addition change of neutron polarisation in the scattering process):

the nominator is the number of scattered neutrons per second into angle element dΩ with energies between E' and E'+dE' and can be written as W(k,k')dN', where

W(k,k') … transition probability per time from plane incoming wave with vector k to scattered wave with vector k', it is given by Fermis golden rule as 2πℏ Σ_σ,k<k' Σ_σ,k<k' |<i|<k|<sn||Hint|sn'|<f>|<k'|

dN' ………number of scattered states in energy and Ω element dE'dΩ around k', this can be calculated by imaging the neutron states as plane wave states in a (large) periodicity volume V=L^3

the possible states are plane wave states with wave vectors (kx,ky,kz)=(nx,ny,nz) 2π/L, the nx,ny,nz being integer numbers.Any summation over these plane wave states Σ_nx,ny,nz can for large periodicity Volume be written as an integral using the relation 1=Ldx/2π Ldy/2π Ldz/2π, which in the integral becomes [f(...)]Vd(k'/2π)^3, from this we conclude that
dN'= Vd(k'/2π)^3=Vk'^2d'k'dΩ'dE'

The denominator consists of dE'dΩ times j,

j …. The neutron flux of incoming neutrons, which can be written as j=ν/V=ℏk/MV (ν is neutron velocity, M neutron mass)

these ingredients we use to obtain the Master equation on the next slide …
In the Master equation the Fourier transform of the interaction Hamiltonian has been defined, i.e. the integration over the spatial neutron coordinates in the wave function has been carried out (see formula on the next slide).

We now proceed with unpolarised neutron beams, so the probabilities for all spin states $P_{sn}$ are equal, we will use

1) $P_{sn} = 1/2$

2) $1 = \sum_{sn} |sn><sn|$

3) $\sum_{sn} <sn|s_n^{\alpha}\beta|sn>|sn><sn| = \delta_{\alpha\beta}/4$, here $\alpha\beta$ refer to spatial coordinates $x,y,z$ of the spin vector $s_n$

Thus we will get rid of the spin coordinates in the Master equation in the next two slides …
Interaction of Neutrons with Matter

Here we write down explicit expressions for the interaction of the neutron with matter. Neutrons interact with the nuclei and with the electrons.

The nuclear interaction is given by the nuclear potential, which in comparison to the neutron wavelength is well localised in space and can be replaced by a deltafunction times a constant. These constant, however, may depend on the orientation of the nuclear spin relative to the neutron spin $I$ due to an exchange interaction. Probably the concept of exchange interaction is not familiar to some of you and I mention here without proof that exchange interactions result from the requirement that the wave function of identical particles should be antisymmetric in the particle coordinates (Pauli principle). If one is lazy and does not want to do this antisymmetrisation of the wave function (in our case we are lazy and do not want to bother that the wave function of the nuclear neutrons and that of our neutron being scattered have to be antisymmetric), Heisenberg has invented a nice trick: we can calculate everything with product wave function, just as if the neutrons were distinguishable, but we have to introduce in addition to the other energies involved an exchange interaction, which is given by the product of the spins times a constant. This constant is determined by the overlap of the wave functions. More details can be found in any textbook or lecture on magnetism, e.g. on my homepage ...

The nuclear interaction is easily Fourier transformed due to the deltafunction involved.

Let me turn now to the magnetic interaction, the expression shown here is given in terms of (generalized) electronic momentums in the sample ($P_e$) and the magnetic vector potential $A$. It can be derived in the following way: we consider the change of electronic energy due to the magnetic field created by the neutron (one can also look at the change of the neutron energy due to the magnetic field created by the electrons and get the same result). A magnetic field will give rise to a Zeeman term (last term in the above equation) involving the electronic spin. In addition the magnetic field created by the neutron will change the spatial movement of the electrons and has to be added to the magnetic Vector potential in the kinetic energy term. Please note, that in Hamilton mechanics the kinetic energy term in the presence of magnetic field has to be written in terms of a generalized momentum $P$ (which is the Lagrange conjugate variable of the space coordinate) and is nothing but the momentum of the electrons minus $e/c$ times the magnetic Vector potential $A$. Thus inserting a magnetic field will not change the kinetic energy (as known from electromagnetism). The difference between kinetic energy term with the field created by the neutron and without gives the corresponding term in the interaction Hamiltonian. Note the sum is over all electrons “e” in the sample.

In the next step in a formal way the total interaction is written in terms of a neutron spin dependent part (blue) and a spin independent part (yellow) and inserted into the master equation of the previous slide. Then the spin coordinates are eliminated using the formulas given on the previous slide resulting in the first expression on the next slide …
Unpolarised Neutrons - Van Hove Scattering function \( S(Q,\omega) \)

\[
\frac{d^2 \sigma}{dQdE} = \frac{k^4}{4\pi^2} \left( \frac{M}{2\hbar^2} \right)^2 \delta(\hbar\omega + E_i - E_f) \sum_{ij} P_i \langle i \mid \hat{\beta} \mid f \rangle^2 + \langle i \mid \hat{\alpha} \mid f \rangle \cdot \langle f \mid \hat{\alpha} \mid i \rangle
\]

- for the following we assume that there is no nuclear order - \(<\hat{I}\>=0\):

\[
\frac{d^2 \sigma}{dQdE} = \frac{N k^4}{k} \left( \frac{\hbar c^2}{m^2 c^2} \right)^2 \sum_{ij} (\delta_{ij} - \hat{Q}_i \hat{Q}_j) S_{ij}^{mag}(\hat{Q},\omega) + \frac{N k^4}{k} S_{nm}^{mag}(\hat{Q},\omega)
\]

\[
S_{ij}^{mag}(\hat{Q},\omega) = \frac{1}{2\pi \hbar} \int_0^\infty dt e^{i\omega t} \frac{1}{N} \sum_{ij} \left\{ \frac{1}{2} gF(Q)_i \frac{1}{2} gF(Q)_j \right\} < J_{j\omega} (t) e^{-i\hat{Q} \cdot \hat{Q}_{j\omega} (t)} J_{j\omega} (0) e^{i\hat{Q} \cdot \hat{Q}_{j\omega} (0)} >
\]

\[
S_{nm}^{mag}(\hat{Q},\omega) = \frac{1}{2\pi \hbar} \int_0^\infty dt e^{i\omega t} \frac{1}{N} \sum_{ij} (b_i^* b_j^* + b_i^* b_j^* + \frac{1}{2} \delta_{ij} J_j (I_j + 1)) < e^{-i\hat{Q} \cdot \hat{Q}_{j\omega} (t)} e^{i\hat{Q} \cdot \hat{Q}_{j\omega} (0)} >
\]

Splitting of \( S \) into elastic and inelastic part

\[
\hat{R}_j (t) = \hat{R}_j + \hat{u}_j (t)
\]

\[
S_{nuc} = S_{nuc}^{el} + S_{nuc}^{inel}
\]

\[
S_{nuc}^{el} = \delta(\hbar\omega) \frac{1}{N} \sum_{ij} \left\{ b_i^* b_j^* + b_i^* b_j^* + \frac{1}{2} \delta_{ij} J_j (I_j + 1) \right\} < J_{j\omega} (t) > e^{-i\hat{Q} \cdot \hat{Q}_{j\omega} (t)} e^{i\hat{Q} \cdot \hat{Q}_{j\omega} (0)} e^{-\hat{W}_j - \hat{W}_j'}
\]

\[
S_{nuc}^{inel} = \delta(\hbar\omega) \frac{1}{N} \sum_{ij} \left\{ b_i^* b_j^* + b_i^* b_j^* + \frac{1}{2} \delta_{ij} J_j (I_j + 1) \right\} < J_{j\omega} (t) > e^{-i\hat{Q} \cdot \hat{Q}_{j\omega} (t)} e^{i\hat{Q} \cdot \hat{Q}_{j\omega} (0)} e^{-\hat{W}_j - \hat{W}_j'}
\]

We now turn to analyse the double differential cross section in terms of vanHove scattering functions \( S \) for the magnetic and the nuclear part, which both can be written as a sum of elastic and inelastic contributions. In doing this we write the matrix elements in the Heisenberg representation of quantum mechanics, which takes the time dependence from the state vector and puts it to the operators, in our case \( R \) and \( J \) (see textbook on quantum mechanics for further details). The next step is to write the positional operators \( R_j(t) \) in terms of the equilibrium position (\( R_j \), a number vector) and the deviation \( u_j(t) \) (a Vector operator). When considering elastic scattering function, we can consider the effect of the \( u_j \) by assuming an uncorrelated movement of the different atoms (i.e. neglecting phononic correlations) in an harmonic oscillator potential. Even without the more rigorous proof (which is available but more complicated) we can see that

\[
<exp(-i u_j Q)> \sim 1 - <i u_j q> - 0.5 <u_j Q > + ... \sim 1 - 0.5 <u_j Q>^2 \sim exp(-<u_j Q>^2)/2 = exp(-W_j)
\]

In case of isotropy of the Einstein oscillators the \( W_j \) can be simplified to \( W_j = <u_j Q>^2>/2 = Q^2 <u_j^2>/6 \)
A short Excursion to Fourier and Delta Functions ....

\[ f(x) = \sum_{n=0}^{\infty} f_n e^{i n x / L} \] ...

\[ f(x) = \int_{-L/2}^{L/2} f(x') e^{-i n x' / L} dx' \]

\[ \delta(x - x') = \frac{1}{L} \sum_{n=0}^{\infty} e^{i n (x - x') / L} \]

\[ \delta(cx) = \frac{\delta(x)}{c} \]

\[ q_a = \frac{2 \pi \sigma}{L} \sum_{n=0}^{\infty} e^{i n a} = \frac{2 \pi}{a} \delta(q) \]

it follows by extending the range of x to more than \(-L/2 \ldots L/2\) and going to 3 dimensions \((v_0\) the unit cell volume):

\[ \sum_{kk'} e^{-i q \cdot \vec{r}_k - i \vec{r}_{k'}} = N_G \frac{(2 \pi)^3}{v_0} \sum_{\text{rec. lat. } \vec{t}} \delta(\vec{Q} - \vec{q}) \]
Using the formulas of the previous slide we discuss now the elastic scattering, first the nuclear contribution.

A speciality of neutron scattering already mentioned by Helmut Rauch is the incoherent scattering contribution which arises from averaging the scattering cross section over different possible isotope distribution in the sample. This averaging process we indicate by a horizontal bar above the symbols. We note that the average of a product of scattering lengths has to be done with great care, because for the same atom the average of the square of the scattering length is not equal to the scattering length average squared (i.e. \( <b>^2 \neq <b^2> \)), therefore, \( <bj^* bj'> = <bj'^* bj> \) - \( \delta_{jj'} \). This leads to the isotope incoherent scattering. Even in the case of one isotope there is in addition the spin incoherent scattering arising from the nuclear spins, which are not oriented (unless there is nuclear order at very low temperatures, which may occur below a few mK).
Magnetic Diffraction

\[ S_{\text{nuc\ coh}}^{\text{el}} = \delta(h\omega) \frac{1}{N} \sum_{ij} b_j^* b_i e^{-i\hat{Q}_j \cdot R_i} e^{i\hat{Q}_i \cdot R_j} \]

\[ S_{\text{mag}}^{\text{el}} = \delta(h\omega) \frac{1}{N} \sum_{ij} \left\{ \frac{1}{2} g F(Q) \right\}_j < J_{j\alpha} > T \left\{ \frac{1}{2} g F(Q) \right\}_j < J_{j\beta} > T e^{-i\hat{Q}_j \cdot R_i} e^{i\hat{Q}_i \cdot R_j} \]

\[ \frac{d^2\sigma}{d\Omega dE} = N k' \left( \frac{\hbar e^2}{mc^2} \right)^2 \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) S^{\alpha\beta}_{\text{mag}}(\hat{Q}, \omega) + N k' S_{\text{nuc}}(\hat{Q}, \omega) \]

Difference to nuclear scattering:

- Formfactor \( \left\{ \frac{1}{2} g F(Q) \right\}_j \) ... no magnetic signal at high angles
- Polarisationfactor \( (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \) ... only moment components normal to \( Q \) contribute
Atomic Lattice

Magnetic Lattice

ferro

antiferro
Atomic Lattice

Magnetic Lattice

ferro

antiferro
Atomic Lattice

Magnetic Lattice

ferro

antiferro
In 1949 Shull showed the magnetic structure of the MnO crystal, which led to the discovery of antiferromagnetism (where the magnetic moments of some atoms point up and some point down).
Dipole Approximation (small Q): 

\[ F(Q) = \langle j_0(Q) \rangle + \frac{2 - g}{g} \langle j_2(Q) \rangle \]

... in Shulls data we see that the magnetic intensity is strongest at small scattering angle and decays at higher angles due to the magnetic form factor.
Arrangement of Magnetic Moments in Matter

- Paramagnet

- Ferromagnet

- Antiferromagnet

And many more ....
Ferrimagnet, Helimagnet, Spinglass ...collinear, commensurate etc.
In the next few slides I show, what nowadays is usually done automatically by a computer program. First, the size of the magnetic supercell of an antiferromagnet has been determined from the position of magnetic satellite reflections, which appear below the Neel temperature. Then the moment orientation can be determined by fitting the magnetic diffraction pattern. The computer calculates for every magnetic reflection the magnetic structure factor and from this the magnetic intensity. Then by convolution with the instrumental resolution a diffraction pattern is calculated which can be compared to the experimental pattern for different moment orientations … have a look at the subsequent slides on how this works.
\[ \text{GdCu}_2 \quad T_N = 42 \text{ K} \quad M \perp [010] \]

\[ T_R = 10 \text{ K} \quad q = (2/3 \ 1 \ 0) \]

**Magnetic Structure from Neutron Scattering**

Experimental data D4, ILL

Calculation done by McPhase
GdCu$_2$  \( T_N = 42 \text{ K} \)  \( M \perp [010] \)
\( T_R = 10 \text{ K} \)  \( q = (2/3 1 0) \)

Magnetic Structure from Neutron Scattering

Experimental data D4, ILL
Calculation done by McPhase

$\text{GdCu}_2$  $T_N = 42 \text{ K}$  $M \perp [010]$  
$T_R = 10 \text{ K}$  $q = (2/3 \ 1 \ 0)$

**Magnetic Structure from Neutron Scattering**

Experimental data D4, ILL
Calculation done by McPhase

GdCu$_2$  

$T_N = 42$ K  \( M \perp [010]\) 

$T_R = 10$ K  \( q = (2/3 1 0)\) 

Magnetic Structure from Neutron Scattering


Experimental data D4, ILL
Calculation done by McPhase
The quality of a fit is usually described by parameters such as the Rp value …
Another example of magnetic diffraction: when complex magnetic phases have to be studied, nowadays cryomagnets can be mounted on diffractometers and spectrometers. Here I show a vertical field magnet for extremely high fields. In such a split coil system fields up to 15/17 T may be produced. Using such a setup, the diffraction can be done on single crystals and the different magnetic structures which can be stabilised by variation of temperature and magnetic field can be studied.
Complex Structures

Experimental data TAS6, Riso Loewenhaupt, Z. Phys. (1996) 499

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NESY Winter School 2009
Complex Structures

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Complex Structures

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A recent investigation during my first months in Oxford concerned the dipole approximation of the magnetic form factor. In the dipole approximation only the total dipolar moment on each magnetic ion enters the cross section. However, in many atoms the dipolar moment is not homogeneously distributed in the unfilled shell. Due to the crystal electric field generated by neighboring atoms the magnetic moment density is usually highly anisotropic. The neutrons in general are sensitive to the Fourier transform of this magnetic moment density in the atom, here I denote it by $M(Q)$. In the literature frequently also the scattering operator $Q$ is used, which must not be confused with the momentum transfer.
In the following I will show what effect going beyond the dipole approximation has in the interpretation of magnetic diffraction pattern.
CePd$_2$Si$_2$

*bc* ThCr$_2$Si$_2$ structure
Space group I4/mmm
Ce$^{3+}$ (4f1) J=5/2
$T_N$=8.5 K
q=(1/2 1/2 0), $M=0.66 \mu_B$/Ce

$q=(1/2 1/2 0), M=0.66 \mu_B$/Ce

Comparison to experiment

\[
\frac{|\text{FM}|^2 - |\text{FM dip}|^2}{|\text{FM dip}|^2} \times 100 \%
\]

Goodness of fit:

$R_p^{\text{dip}}=15.6\%$

$R_p^{\text{bey}}=8.4 \%$

($R_p^{\text{nuc}}=7.3\%$)

Going beyond the dipolar approximation a clear improvement of the description of the experimental data can be obtained, as is shown by the lower Rp value.
NdBa$_2$Cu$_3$O$_{6.97}$

*superconductor $T_c=96$K*

*orth* YBa$_2$Cu$_3$O$_{7-x}$ structure

Space group Pmmm

Nd$^{3+}$ (4f$^3$) $J=9/2$

$T_N=0.6$ K

d($\frac{1}{2} \frac{1}{2} \frac{1}{2}$), $M=1.4$ $\mu_B$/Nd

---

... using the *dipole approximation* may lead to a wrong magnetic structure!

| $h$ | $k$ | $l$ | $|Q|$ | $I_{obs} \pm \sigma_{obs}$ | $I_{mag}$ | $I_{mag}$ |
|-----|-----|-----|------|-----------------|-----------|-----------|
|     |     |     | (1/Å) |                | $\theta = 0$ | $\theta = 12^\circ$ |
| 0.5 | 0.5 | 0.5 | 1.1749 | 115±4          | 110       | 111       |
| 0.5 | 0.5 | 1.5 | 1.3981 | 84 ±3          | 81        | 78        |
| 0.5 | 0.5 | 2.5 | 1.5017 | 50 ±1          | 49        | 49        |

In NdBaCuO a wrong magnetic structure was published, because A. Boothroyd used the dipole approximation for the form factor in the fit of the experimental data. Therefore in future we should definitely use always the exact calculation to fit magnetic diffraction data and avoid misinterpretation of the experimental data!
Inelastic Magnetic Scattering

Here I show again the different methods for investigating excitations in matter. The red ellipses indicate that for magnetic excitations many methods are not applicable and we are left with neutrons, NMR (nuclear magnetic resonance) and muSR (muon spin resonance). Thus for investigation of magnetism in matter neutrons are absolutely necessary. This is frequently ignored by many people discussing on whether a new synchotron or a new neutron source should be built. Please note that magnetism is important for almost all elements in the periodic table, even the form of the periodic table itself cannot be explained without considering the spin of the electrons. It is tempting to neglect the spin degrees of freedom in diamagnetic materials, which we frequently find in nature, i.e. in biology and chemistry and beautiful science can be done without spin. However, at some stage also in these studies one may find, that spin is important, and then we need neutrons to investigate it.
Here the principle of a three axis spectrometer is shown …
PANDA – TAS for Polarized Neutrons at the FRM-II, Munich
PANDA – TAS for Polarized Neutrons at the FRM-II, Munich

beam-channel
Cabin with computer work-places and electronics
monochromator-shielding with platform
secondary spectrometer with surrounding radioprotection, 15 Tesla / 30mK Cryomagnet
… some parts of PANDA
Movement of Atoms [Sound, Phonons]

Brockhouse 1950...

The Nobel Prize in Physics 1994

Phonon Spectroscopy: 1) neutrons
2) high resolution X-rays

E \quad \pi/a

Q

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The simplest model for magnetic excitations in solids – however it is not correct, as experiments on the next slide show … the reason is, that changing one spin will effect the neighbors, which tend to be oriented parallel to this spin because of the exchange interaction, next slide shows what I mean.
\[ H = -\frac{1}{2} \sum_{ij} J(ij) S_i \cdot S_j \]

… The \( q \) dependence of magnetic excitations shows dispersion, this confirms the spinwave model for magnetic excitations, see next slide
Movement of Spins - Magnons

\[ H = -\frac{1}{2} \sum_{ij} J(ij) S_i \cdot S_j \]

Bohn et. al.
PRB 22 (1980) 5447
We put charges in the vicinity of a magnetic ion, this creates an electric field, the so-called crystal field. It deforms the charge density associated with the magnetic electrons. In quantum mechanics this leads to a splitting of the degenerate magnetic ground state. Neutrons can trigger excitations between these split states and thus change the charge density (although the interaction between the neutron and the electron is only magnetic), note that with each state a different charge density is associated – see next slides for an example...

Note that this is a simple picture. It may happen that the change in the charge density on one ion will change the crystal field on the neighboring ion and consequently also the charge density on the neighbor. This can be described by an two ion interaction involving higher order (e.g. quadrupolar) moments. As in the case of magnetic excitations, such an interaction will lead to dispersive modes characterising a correlated change in the charge density. I will show later how this idea leads to the concept of orbital excitations, orbitons.
A crystal field spectrum of a magnetic ion … using this spectrum, the crystal electric field has been determined …
For each state the charge density is different…. The different crystal field states are populated when increasing the temperature. Thus at high temperature the charge density gets spherical. This leads to an anisotropic contribution to the thermal expansion of the solid. Thus neutrons may help to understand bulk properties.
Inelastic scattering is complicated. This slide outlines the basic concept for the calculation of magnetic excitations. A central equation is the so called “fluctuation dissipation theorem” which relates the dynamical susceptibility $\chi$ to the scattering function $S$.
An example of a study of magnetic excitations in different magnetic phases by applying magnetic a magnetic field on a three axis spectrometer. The dispersion plots show many modes, the number of modes is equal to the number of magnetic ions in the magnetic supercell times the transitions between the levels on these ions. For Nd at low temperature only the crystal field groundstate doublet has to be considered, thus in this case we have only one transition per ion and the number of modes is equal to the number of Nd ions in the magnetic supercell. All data can be described by a unique set of exchange interaction parameters for this system. The calculation of the dispersion is far from trivial and has been done using the formalism outlined on the previous slide. The green lines show the results of these model calculations, the point size corresponds to the intensity of the mode. Experimental data was obtained by energy scans at constant wave vector transfer Q. From the maxima in the spectra the position of the modes in energy was determined and is shown by the symbols.
Coming back to what I have mentioned along with the introduction of the crystal field concept I show, that besides phonons and spinwaves I believe in the existence of orbital excitations. Currently it is still a matter of believe, because we do not have enough experimental evidence for this type of excitations. The reason is, that it is difficult to distinguish between orbitons and magnons. This is in contrast to phonons and magnons, where the two types of excitations can clearly be distinguished due to the different interaction (nuclear, electronic) leading to a different q dependence of intensity. Also polarised neutron experiments can be used to distinguish between phonons and magnons. For orbitons, the only difference to magnons is, that the interaction which leads to the dispersion is not bilinear but of higher order for the orbitons. However, in some cases it may be possible to establish an orbiton, this is when we observe a large dispersion of magnetic excitations and know, that the magnetic interaction must be small (this we may conclude from a very low magnetic ordering temperature). Then only higher order interactions can be the reason for the large dispersion. Some cases in literature and some own experiments on PrCu2 indicate the existence of orbitons. Further research is strongly needed to learn more about this type of excitations.
Summary

• Magnetic Diffraction
• Magnetic Structures
• *Caveat* on using the Dipole Approx.

• Magnetic Spectroscopy
• Magnons (Spin Waves)
• Crystal Field Excitations
• Orbitons
McPhase

A Mean field monte Carlo
PHASE
diagram program

Martin Rotter, University of Oxford
This software suite is the result of more than 10 years programming. It allows the evaluation of magnetic properties including neutron scattering cross sections.
McPhase runs on Linux & Windows
it is freeware

www.mcphase.de

Magnetostriction

and much more....
Important Publications referencing McPhase:


Thanks to ......

M. Doerr, M. Loewenhaupt, TU-Dresden
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