Bridging Length Scales in Magnetism – Diffuse Scattering from the Atomic to the Mesoscale

812. WE-Heraeus-Seminar

16 - 19 June 2024

at the
Physikzentrum, Bad Honnef, Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 812. WE-Heraeus-Seminar:

This WE-Heraeus seminar focuses on the technique of magnetic small-angle neutron scattering(SANS) and its extension towards a unified description of diffuse scattering from the atomic to the mesoscale. Magnetic SANS is well established to elucidate the magnetic structure of a wealth of different systems as diverse as from nanotextured materials all the way to emergent spin textures of strongly correlated electron systems and superconductors. An equally rich group of material classes is also characterized by the absence of long-range magnetic order and – in turn – by their diffuse scattering signature, however, on an atomic length scale. Their magnetic structure is typically characterized by disorder introduced by frustrated or competeing magnetic interactions or the proximity to quantum criticality or emergent superconductivity. It has only recently been discovered, that in fact, a large overlap exists between these rather separated communities: Experiments showed that the diffuse scattering signatures of the aforementioned disordered quantum spin systems can reach far into the mesoscopic nm-regime of magnetic SANS. Likewise, atomic scale order and disorder phenomena become more and more relevant for nanotextured systems, which may benefit from insight into the concepts of diffuse magnetic scattering.

We intend to gather scientists working on the different applications of magnetic SANS and diffuse scattering and providing a stage for intra- and interdisciplinary scientific exchange. We expect that both scientists from communities will strongly benefit from such an interaction by sharing the latest trends and concepts that may become relevant in theory and experiment.

Introduction

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Introduction

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Registration:

Marion Reisinger (WE Heraeus Foundation)
at the Physikzentrum, reception office
Sunday (17:00 h – 21:00 h) and Monday morning

Program

Program

Sunday, 16 June 2024

17:00 – 21:00	Registration	
From 18:00	*BUFFET SUPPER*	
19:30 – 19:45	Scientific organizers	**Opening and Welcome**
19:45 – 20:30	Collin Broholm	**Diffuse neutron scattering from frustrated magnets**

Monday, 17 June 2024

08:00 – 09:00	*BREAKFAST*	
09:00 – 09:45	Johanna Jochum	**Dynamics of diffusely scattering magnetic phenomena**
09:45 – 10:15	Cedric Gommes	**Stochastic models for small-angle scattering analysis in disordered systems**
10:15 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Joseph Paddison	**Understanding Spin Textures Using Magnetic Diffuse Scattering**
11:45 – 12:15	Lukas Beddrich	**The influence of dipolar interactions on the critical dynamics in Ni investigated by high-resolution neutron spectroscopy**
12:15	*LUNCH*	
14:30 – 15:15	Annika Stellhorn	**Polarized SANS and GISANS at the ESS**
15:15 – 15:45	**Posterflash**	
15:45 – 16:30	*COFFEE BREAK*	
16:30 – 17:30	**Poster Session**	
18:30	*DINNER*	

Program

Tuesday, 18 June 2024

08:00 – 09:00	*BREAKFAST*	
09:00 – 09:45	Alexander Tsirlin	**Frustration vs. randomness in spin-1/2 triangular antiferromagnets**
09:45 – 10:15	Robert Georgii	**A Time-of-flight Crystal Analyzer Spectrometer for FRM II**
10:15 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Robert Cubitt	**Going to Great Lengths in Superconductivity**
11:45 – 12:15	Elizabeth Martín Jefremovas	**Magnetic super-structures in RCu_2 (R ≡ Nd, Tb) nanoparticle ensembles**
12:15	*LUNCH*	
14:30 – 15:15	Yixi Su	**Highly tunable magnetism in magnetic kagome metals RMn_6Sn_6**
15:15 – 15:30	Ivan Titov	**Novel Angular Anisotropy in Polarized Magnetic Small-Angle Neutron Scattering**
15:30 – 15:45	Steven Parnell	**Probing longer magnetic correlation lengths using spin echo modulated small angle neutron scattering (SEMSANS)**
15:45 – 16:30	*COFFEE BREAK*	
16:30 – 17:15	Henrik M. Rønnow	**Neutron studies of $SrCu_2(BO_3)_2$ under extreme conditions – a fruit fly for quantum many body physics**
17:15 – 18:00	Elizabeth Blackburn	**Magnetic dynamics in the small angle regime**
18:30	*HERAEUS - DINNER* *(social event with cold & warm buffet and complimentary drinks)*	

Program

Wednesday, 19 June 2024

08:00 – 09:00	*BREAKFAST*	
09:00 – 09:45	Andrew Wildes	**Neutron diffuse scattering, and disorder on the atomic scale**
09:45 – 10:00	Nahal Rouzbeh	**Magnetic Morphology and Exchange-Coupling in Cobalt-Doped Iron Oxide Core-Shell Nanoparticles**
10:00 – 10:15	Michael Philipp Adams	**Signature of surface anisotropy in the spin-flip neutron scattering cross section of spherical nanoparticles: Atomistic simulations and analytical theory**
10:15 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Alex Backs	**Magnetic Neutron Imaging – Methods & Applications**
11:45 – 12:15	Ahmed Alshemi	**Investigating the superconducting state of 2H-NbS_2 as seen by the vortex lattice**
12:15 – 14:30	*LUNCH*	

End of the seminar and departure

Posters

Poster Session, Monday 17 June 2024, 16:30 h

Jonathan Gustavo Acosta Ramón	**Influence of randomness in 3D and 2D magnetic frustrated systems seen by neutron scattering**
Diego Alba Venero	**Development of magnetic SANS at ISIS**
Jan Blessing	**Machine learning Based Data Analysis for Small Angle Neutron Scattering**
Gregor Bulitta	**Machine learning based Optimization of Measurement Strategies for Small Angle Neutron Scattering**
Madhu Ghanathe	**Magnetic field dependent neutron diffraction studies of polycrystalline $Ho_3Fe_5O_{12}$**
Chun-Hao Huang	**Magnetic order in the quasi-one-dimensional quantum magnet candidate compound $NdOCa_4(BO_{3)3}$**
Paul Kamminga	**Tuning Atomistic Disorder in Nanoparticles**
Gaurav Kanu	**Spin order and disorder at interfaces in nanoscale magnets probed by neutron scattering**
Emmanuel Kentzinger	**The high-brilliance laboratory X-ray diffractometer GALAXI: from mesoscopic to interatomic length scales**
Vlad Kuchkin	**Bloch points in classical and quantum magnetic systems**
Stefan Liscak	**Signature of magnetic skyrmions in the chiral function**
Denis Mettus	**Portable devices for extending resolution of small-angle neutron scattering instrument at FRM-II**
Asmaa Qdemat	**Characterization of Magnetic Multilayers Deposited onto Nanosphere Arrays Using Grazing Incidence Small-Angle X-ray Scattering (GISAXS)**

Poster Session, Monday 17 June 2024, 16:30 h

Venus Rai	**Magnetic microstructure of nanocrystalline Fe-Nb-B alloys as seen by small-angle neutron and X-ray scattering**
Leonhard Rochels	**Spin Correlations in Assemblies of Iron Oxide Nanoparticles**
Evelyn Pratami Sinaga	**Neutron scattering signature of the Dzyaloshinskii-Moriya interaction in nanoparticles**
Yung-Hsiang Tung	**Bridging experimental insights and theoretical models to decipher the exchange interactions in $CaCu_3Ti_4O_{12}$**
Tereza Vaclavu	**The local structure of iron oxide nanoparticles upon lithiation**

Abstracts of Lectures

(in alphabetical order)

Signature of surface anisotropy in the spin-flip neutron scattering cross section of spherical nanoparticles: Atomistic simulations and analytical theory

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We investigate the signature of magnetic surface anisotropy in nanoparticles in their spin-flip neutron scattering cross section. Taking into account the isotropic exchange interaction, an external magnetic field, a uniaxial or cubic magnetic anisotropy for the particle's core, and several models for the surface anisotropy (Néel, conventional, random), we compute the spin-flip small-angle neutron scattering (SANS) cross section from the equilibrium spin structures obtained using the Landau-Lifshitz equation. The sign of the surface anisotropy constant, which is related to the appearance of tangential- or radial-like spin textures, can be distinguished from the momentum-transfer dependence of the spin-flip signal. The data cannot be described by the well-known and often-used analytical expressions for uniformly magnetized spherical or core-shell particles, in particular at remanence or at the coercive field. Based on a second-order polynomial expansion for the magnetization vector field, we develop a novel minimal model for the azimuthally averaged magnetic SANS cross section. The theoretical expression considers a general magnetization inhomogeneity and is not restricted to the presence of surface anisotropy. It is shown that the model describes very well our simulation data as well as more complex spin patterns such as vortexlike structures. Only seven expansion coefficients and some basis functions are sufficient to describe the scattering behavior of a very large number of atomic spins.

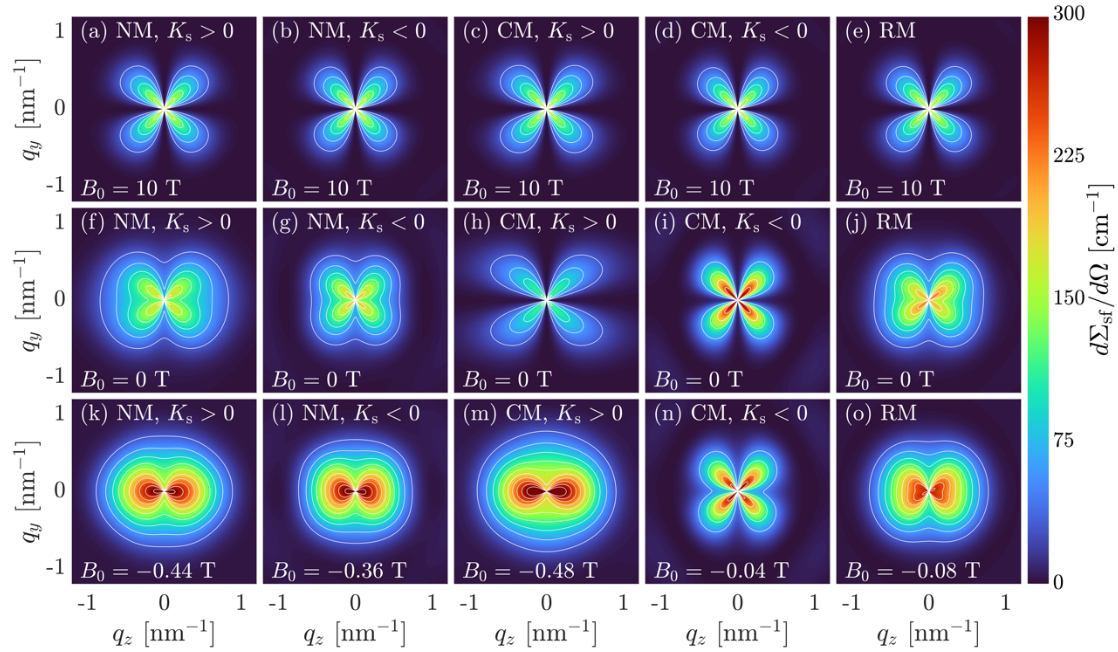

Figure 1: Spin-Flip SANS cross sections for nanoparticles with different surface anisotropies [1].

References

[1] M. P. Adams *et al.*, Phys. Rev. B **109**, 024429 (2024).

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Investigating the superconducting state of 2*H*-NbS_2 as seen by the vortex lattice

Ahmed Alshemi[1], Emma Campillo[1], Edward M. Forgan[2], Robert Cubitt[3], Mahmoud Abdel-Hafiez[4] and Elizabeth Blackburn[1]

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Transition metal dichalcogenides have sparked a lot of interest as they display several electronic orders, including charge density waves, Mott-insulating phases and superconductivity. The family of 2*H*-MX_2 (M = Nb, Ti, Ta; X = S, Se) have similar electronic band structures in the normal state. Within this family, 2*H*-NbS_2 stands out as the only one in which a CDW phase has not been observed. Furthermore, it has been proposed as a host for the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconducting state based on torque magnetometry, specific heat and thermal expansion measurements when the field is precisely perpendicular to the **c**-axis [1]. This implies that there is a strong anisotropy in the superconducting properties in and out of the basal plane.

In our study, we delve into the superconducting properties of 2*H*-NbS_2, a classic anisotropic multi-band superconductor that is currently under much investigation due to the dramatic changes seen when high magnetic fields are aligned parallel to its hexagonal niobium planes. Using small-angle neutron scattering as a bulk-sensitive technique, we have investigated the vortex lattice in 2*H*-NbS_2 and the effect of the superconducting anisotropy on it by changing the magnetic field orientation relative to the Nb planes. We find no changes in the observed superconducting anisotropy across our measured field range, and furthermore we are able to fit all of the intensities of the measured vortex lattice scattering peaks at all angles with a single geometric mean of the London penetration depths in and out of plane. This is done using the anisotropic London theory, as originally postulated by Thiemann *et al.* [2], with the addition of a core-size exponential cut-of, and our results constitute the first complete validation of this longstanding model. Using this model, we are able to determine the two characteristic superconductor length scales: the penetration depth and the coherence length. Our results point to a predominant sampling of the larger superconducting gap in this material.

References

[1] C. Cho et al., Nature Comm. **12**,3676 (2021).
[2] L. Thiemann et al., PRB. **39**, 11406 (1989).

Magnetic Neutron Imaging – Methods & Applications

A. Backs[1,2], S. Sebold[3], T. Kotte[4], W. T. Lee[2], S. Mühlbauer[3], M. Schulz[3], M. Strobl[5,6] and D. Orlov[2]

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Conventionally, neutron imaging is mainly used as a non-destructive method to study the interior of macroscopic samples by measuring the transmission of neutrons. In recent years, the development of imaging techniques was strongly focused on new contrast mechanisms, to expand neutron imaging to new applications [1]. I will present three examples of advanced imaging techniques which can be used for magnetic studies. These techniques combine the spatial resolution of imaging with **a)** Bragg scattering for diffraction imaging, **b)** diffuse very small angle scattering for neutron grating interferometry, and **c)** neutron spin interactions for polarized imaging.
a) For irregular sample shapes, demagnetization effects can be strong, especially at sharp edges or corners, leading to spatial variations of the effective applied magnetic field. In MnSi, diffraction imaging has been used to show that this effect results in an inhomogeneous transition into the skyrmion phase, solving the question about the origin of an extended transition apparent in other measurements [2].
b) In Superconductors, irregular geometries affect the flux penetration into a sample, creating an inhomogeneous field distribution. In niobium, where a magnetic domain structure is found in the superconducting vortex matter [3,4], this can create a macroscopic separation of this domain state and a homogeneous vortex lattice. The scattering caused by the magnetic domains can be observed in the dark field mode of neutron grating interferometry, clearly differentiating the two magnetic structures.
c) Large magnetic domains in silicon steel sheets can be observed with polarized neutron imaging, where the sample internal field induces spin precession [5]. Measurements give information about the magnetic properties of the domains and allow to study domain growth, movement and merging in an applied magnetic field, including effects from macroscopic inhomogeneities such as grain boundaries.

References

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[5] A. Backs, et al., EPJ Web of Conferences 286, 05003 (2023)

The influence of dipolar interactions on the critical dynamics in Ni investigated by high-resolution neutron spectroscopy

L. Beddrich[1,2], **J. K. Jochum**[1], **S. Säubert**[3, 4], **C. Franz**[2, 5] **and P. Böni**[1]

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Inelastic neutron scattering techniques and the study of spin dynamics in magnetic materials have long driven each other's advancements. Traditionally, studies on ferromagnets like iron and nickel were limited by coarse resolution, even with state-of-the-art instruments. However, employing the modern neutron spectroscopy method MIEZE [1], we probed nickel's spin wave dispersion and paramagnetic spin fluctuations with unprecedented detail at small momentum and energy transfers.

The MIEZE technique, implemented at the resonance spin-echo spectrometer RESEDA, uniquely enables the investigation of magnetic phenomena despite depolarizing samples and environmental conditions [2]. Its versatility allows for studying weak and low-energy magnetic dynamics with reasonable measurement times, thanks to its tolerance for a broad wavelength spectrum and large neutron flux. Recent upgrades to the instrument have improved background suppression, q coverage, and energy resolution.

Analyzing the spin wave dispersion of isotropic ferromagnets using the Holstein-Primakoff theory (HPT) reveals insights into weak dipolar interactions [3]. The dispersion should be quadratic for a pure Heisenberg-like ferromagnetic system for small q values $E_{SW} \propto q^2$. In contrast, HPT predicts a linear q dependence of the dispersion due to the long-range dipolar interactions between the magnetic moments. In addition to the dispersion, influences on the lifetime of critical fluctuations above T_C are also expected because the length scale q_D^{-1} should enter the dynamical scaling function as a second scaling variable and separate longitudinal from transversal modes [4].

References

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[3] T. Holstein *et al.*, Phys. Rev., **58**, 1098 (1940)
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Magnetic dynamics in the small angle regime

Elizabeth Blackburn[1]

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The short range order often captured by diffuse scattering is seen in a huge variety of materials. From the fluctuation-dissipation theorem, we expect that this short-range scattering may display dynamics on a range of time scales, depending on the specific origin of the diffuse scattering signal. This has been explored extensively using techniques like neutron techniques like backscattering and neutron spin echo, as well as X-ray techniques like speckle spectroscopy, particularly for studies of polymers, and in the magnetic domain, spin glasses. In the small angle regime, the interaction of the neutron with magnetic fields leads to additional inelastic features, which will be illustrated using examples from superconductors and chiral magnetic structures.

Diffuse neutron scattering from frustrated magnets

Collin Broholm

Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD, USA

I will provide an overview of the role of diffuse magnetic neutron scattering in the exploration and understanding of frustrated magnets. After an introduction to the theoretical background, I will focus on classical and quantum magnetism on the pyrochlore lattice and on honeycomb related lattices.

On the pyrochlore lattice I discuss the relation between diffuse scattering and the monopolar description of spin ice including experiments probing time dependent scattering from $Ho_2Ti_2O_7$[1]. I then discuss the near isotropic spin-1 antiferromagnetism of $NaCaNi_2F_7$[2] and interpretations of its diffuse scattering.

In two dimensions I will discuss frustrated magnetism on the honeycomb lattice resulting from bond dependent Kitaev interactions and competing longer range interactions [3]. This will lead to a discussion of the role of itinerant electrons and lattice distortions in frustrated magnets as exemplified by $(V_{1-x}Cr_x)_2O_3$[4].

Throughout the talk I will highlight the great improvements in neutron source and instrumentation performance that continue to enable new insights in fundamental aspects of many body physics and magnetism.

References

[1] "Monopolar and dipolar relaxation in spin ice $Ho_2Ti_2O_7$," Yishu Wang, T. Reeder, Y. Karaki, J. Kindervater, T. Halloran, N. Maliszewskyj, Yiming Qiu, J. A. Rodriguez, S. Gladchenko, S. M. Koohpayeh, S. Nakatsuji, and C. Broholm, Sci. Adv. **16**, eabg0908, (2021).

[2] "Continuum of quantum fluctuations in a three-dimensional S=1 Heisenberg magnet," K. W. Plumb, H. J. Changlani, A. Scheie, Shu Zhang, J. W. Krizan, J. A. Rodriguez-Rivera, Yiming Qiu, B. Winn, R. J. Cava & C. Broholm, Nature Physics 15, 54-59 (2019).

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Going to Great Lengths in Superconductivity

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Quantisation of magnetic flux in type II superconductors is a source of a rich area of physics where magnetic vortex structures are formed on the scale of 10's of nm in very high fields to 10's of microns in low fields. These supercurrent vortices normally repel each other as the circulating currents interact with the quantised flux but in special cases this interaction is attractive. When this happens the local field, determined by the mean distance between vortices, is locked in and the only way the system can expel flux at low applied fields is to break up into two phases, one with a fixed local field and the other a pure Meissner state with no field at all. The length-scales of the vortex matter regions varies with applied field from a few microns to extending over the whole system at a certain critical field. Bragg peaks from the vortex separation planes are easily measured with small angle neutron scattering but the larger length scales are normally far beyond the limit of this technique. However, diffuse scattering from the domain boundaries does follow a power law which extends into the measurable region. Conventional Porod scattering theory would only allow the extraction of a specific surface, total scattering area normalised by volume. When the structure is aligned, as in this case by the applied magnetic field the specific surface is in fact the reciprocal of the sum of the two characteristic lengths of the system, vortex matter domains and Meissner regions. This allows the measurement of a length-scale up to 50 microns. The analysis technique should be applicable to any two-phase system where the surface boundaries are largely parallel.

A Time-of-flight Crystal Analyzer Spectrometer for FRM II

R. Georgii[1], **C. Herb**[1], **R. Tang**[1] **and J. Voigt**[2]

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Magnetic systems are fertile ground for the design of novel quantum and topologically non-trivial states characterized by exotic excitations. Recent examples include spin chain and square-lattice low-dimensional antiferromagnets, quantum spin liquid candidates, spin-ice compounds, and unusual spin textures. These systems are not only of fundamental interest but may also pave the way to new technologies. For example, skyrmion spin textures open new possibilities for data storage in race track memories [1] and allow for the design of electronic–skyrmionic devices [2]. Key features of the ground state and finite-temperature behavior of a magnetic system are captured by the spectrum of its excitations. All of the aforementioned systems reveal exotic excitations dissimilar to standard magnons that form narrow bands in conventional ferro- and antiferromagnets. The detection of exotic excitations is by far more challenging, as they show broad distribution in the energy and momentum space.

We present a concept for an indirect geometry crystal time-of-flight spectrometer, which we propose for the FRM-II reactor in Garching. Recently, crystal analyzer spectrometers at modern spallation sources have been proposed and are under construction [3,4]. The secondary spectrometers of these instruments are evolutions of the flat cone multi-analyzer for three axis spectrometers (TAS). The instruments will provide exceptional reciprocal space coverage and intensity to map out the excitation landscape in novel materials. We will discuss the benefits of such a time-of-flight primary spectrometer with a large crystal analyzer spectrometer at a continuous neutron source. The dynamical range can be very flexibly matched to the requirements of the experiment without sacrificing the neutron intensity. At the same time, the chopper system allows a quasi-continuous variation of the initial energy resolution. The neutron optic of the proposed instrument employs the novel nested mirror optics [5], which images neutrons from a bright virtual source onto the sample. The spot size of less than 1 cm x 1 cm at the virtual source allows the realization of very short neutron pulses by the choppers, while the small and well-defined spot size at the sample position provides an excellent energy resolution of the secondary spectrometer thanks to the prismatic focusing of the analyzer.

References

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Stochastic models for small-angle scattering analysis in disordered systems

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Developing models to analyze scattering data requires finding a balance between mathematical simplicity and structural realism, which is particularly challenging for disordered systems. Stochastic approaches offer a practical way through these almost antagonistic requirements.

In this presentation I will discuss a variety of stochastic models of disordered structures and I will illustrate their use for scattering data analysis. The examples will focus on small-angle scattering and neutron spin echo data analysis, with applications in porous materials and soft matter.

The presentation will be non-technical, in order to enable discussions with non-specialists, and to explore whether stochastic models developed in other contexts can be useful also for magnetic scattering data analysis.

References

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Dynamics of diffusely scattering magnetic phenomena

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MIEZE (Modulation of Intensity with Zero Effort) is a high-resolution, spin-echo, time-of-flight technique that revolutionizes the study of dynamic magnetic phenomena. Unlike classical neutron spin-echo methods, all beam preparation and spin manipulation occur before the sample, enabling the introduction of depolarizing conditions at the sample position. This unique feature allows for the measurement of magnetic or strongly incoherently scattering samples without signal loss. Moreover, MIEZE allows the application of large magnetic fields at the sample position. This makes MIEZE uniquely well suited for the study of fluctuations at quantum phase transitions and other dynamic magnetic phenomena, including magnon dynamics and relaxation phenomena in disordered magnetic systems such as spin-glasses and spin-ice.

Magnetic super-structures in RCu_2 (R ≡ Nd, Tb) nanoparticle ensembles

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During the last years, the study of non-trivial magnetic structures has been a driving force in solid state Physics, from both fundamental and technological transfer perspectives. More precisely, AF nano–ensembles have attracted a lot of interest, due to the complex magnetic arrangements that can be settled (incommensurability, vorticity, helicity…), so as their inherent advantages with respect to FM [1]. Although there has been a remarkable progress in studying the magnetism at the nanoscale, a clear understanding on how the size reduction modifies the magnetic structure, and the collective interactions, is still under construction. To this aim of understanding the magnetism at the nanoscale, Rare-Earth binary alloys (RCu_2) magnetic nanoparticles (MNPs) are the best platform, on behalf to their high magnetic moment, which *amplifies* the subtle changes happening at the nanoscale [2]. In this work, a detailed study of the magnetic (static) structure, evaluated via powder neutron diffraction (ND) and Small-Angle Neutron Scattering (SANS) of two ensembles of superantiferromagnetic (SAF) MNPs will be presented [3]. Starting with **$NdCu_2$**, the commensurate-incommensurate transition that takes place at T_R = 4.5 K in bulk state vanishes at the MNP regime, indicating the destruction of the helix-like magnetic structure of the bulk. On the other hand, the enhanced RKKY exchanged interactions of **$TbCu_2$** make the AF state exceptionally robust towards size reduction effects, surviving its bulk helix super-structure at the MNPs down to 7 nm. The comparison of both $NdCu_2$ and $TbCu_2$ MNP provides meaningful insights to the robustness of RKKY exchanged interactions against size/dimensionality/symmetry reductions, paving the way towards applications where the combination of a robust AF state plus the nanoparticle dimensionality must be accomplished.

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Understanding Spin Textures Using Magnetic Diffuse Scattering

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Magnetic frustration can suppress conventional magnetic ordering and stabilize unconventional magnetic states. These states can include spin liquids, in which conventional long-range magnetic order is absent. Alternatively, frustration may promote complex long-range magnetic order with novel properties. For example, materials with noncoplanar magnetic structures can show unusual physical properties driven by their nontrivial topology [1]. In this talk, I will discuss how neutron-scattering experiments can be used to identify the magnetic interactions that stabilize spin textures. I will focus on centrosymmetric magnets containing Gd^{3+} ions, such as Gd_2PdSi_3 and $GdRu_2Si_2$, which host multi-**q** skyrmion spin textures under small applied magnetic fields [2,3]. I show how magnetic diffuse scattering measured above the magnetic ordering temperature can identify the magnetic interactions that stabilize the skyrmion phase, establishing a space of magnetic interactions that can promote skyrmion formation [4]. I conclude by discussing the outlook for refinement of magnetic models in interaction space using traditional and machine-learning methods, and I introduce a computer program that can be used to refine interaction models against magnetic diffuse-scattering data [5].

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Probing longer magnetic correlation lengths using spin echo modulated small angle neutron scattering (SEMSANS)

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The inherent flux/collimation arguments in traditional SANS limit the lowest attainable momentum transfer and hence largest length scale that can be observed. By use of the neutron spin we can encode the scattering using a variation of the neutron spin echo technique. Typical spin echo techniques create difficulties for magnetic systems due to the perturbation in the precession caused by the magnetic interactions with the sample.

However using the SEMSANS technique we can observe scattering from magnetic structure without such perturbations as all of the spin manipulations are performed before the sample [1]. This allows samples to be studied as a function of applied magnetic field. We report two different setups at ISIS and HFIR which have now been used to measure correlations in iron, pure and deformed nickel and cobalt samples out to several microns. We discuss the practicalities of such measurements, initial interpretations of the data and how this could be applied to other systems.

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Neutron studies of $SrCu_2(BO_3)_2$ under extreme conditions – a fruit fly for quantum many body physics

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Neutron spectroscopy offer a unique insight into the emergent quantum phases and entangled dynamics in quantum materials.
A textbook example is offered by the compound SrCu2(BO3)2 realizing the theoretical Shastry-Sutherland model, which reveal a plethora of intriguing phenomena including: bosonic flat bands; a zoo of entangled bound states; correlated decay of magnons; valence bond solid of plaquette singlets; a quantum equivalent to the critical point of water; a putative deconfined quantum critical point; fractional magnetization plateaus and bosonic BEC of triplet bound states. Exploring this rich physics in parallel illustrates the challenges and rewards of technological advancements in neutron instrumentation and pushing the capabilities of extreme condition sample environments.
I will present some of the remarkable findings in SrCu2(BO3)2 and illustrate what outstanding questions can be answered through technological advancements like the MORIS programme.

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Magnetic Morphology and Exchange-Coupling in Cobalt-Doped Iron Oxide Core-Shell Nanoparticles

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The exchange coupling in bimagnetic core-shell nanoparticles is a promising pathway to permanent magnetic materials[1]. For iron oxide core-shell nanoparticles, consisting of a wuestite-like particle core and a spinel-type shell, transition metal doping was recently shown to significantly enhance the magnetic anisotropy and exchange coupling[2]. Native iron oxide core-shell nanoparticles synthesized by thermal decomposition of iron oleate typically form as an intermediate through topotaxial oxidation of an initial wuestite phase towards highly defective maghemite[3]. We have recently reported how the combination of such native core-shell nanoparticles (with their alignment of core and shell phases) and cobalt doping leads to a significant enhancement of the exchange pinning between both phases, which is promising for a rational synthesis of nanoparticles with strong coercivity and exchange field. Using magnetic SANS[4,5], we have unambiguously revealed a significant net magnetization even in the wuestite-type nanoparticle core that is commonly presumed antiferromagnetic or paramagnetic at room temperature[6].

In this contribution, we will present the systematic influence of a subtle variation in particle size on the exchange coupling within such native core-shell, Co-doped iron oxide nanoparticles. For freshly synthesized samples with a particle diameter ranging from 8.4 to 9.3 nm, a clear transition from exchange spring to exchange bias behavior is evident. We employ magnetic SANS to elucidate the intraparticle magnetization individually for the wuestite-like particle core and the spinel-type shell and to follow their coupling mechanism.

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Polarized SANS and GISANS at the ESS

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Small-Angle Neutron-Scattering (SANS) with polarization analysis is a powerful technique to investigate magnetic order in hard condensed matter systems on the nanometer and mesoscopic length scales. The high neutron flux expected at the European Spallation Source (ESS), coupled with novel instrumentation that will be supported by a wide variety of sample environments, will be combined with neutron polarization analysis on many instruments [1], enabling exciting new science projects. In this talk, I will present one crucial aspect of a successful scientific study using polarized SANS and its surface-sensitive counterpart Grazing-Incidence SANS (GISANS): The integration of data analysis, data reduction, and instrument work.
Scientifically, the chosen example system is a superconductor(S)/ferromagnet(F) thin film structure with temperature dependent chiral magnetic domain walls [2,3,4]. The instrumentation and data reduction impacts strongly on the interpretation of magnetic chiral structures in the S/F system Nb/FePd. Comparing various different techniques such as polarized GISANS, pi-GISANS, and CD-XRMS, leads to a comprehensive view on the temperature dependent magnetic depth-profile as a function of the perpendicular magnetic anisotropy and can aid in solving the question: which effects are instrumentational, and which are inherent to the sample structure?
For future experiments at the ESS, the above raised question shall be avoided by enabling user-friendly and precise data reduction procedures for polarized (GI)-SANS. I will present the status of polarized (GI)-SANS workflow protocols using the data reduction software Scipp [5], together with updates on the data analysis of magnetic SANS data using the SasView software [6].

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Highly tunable magnetism in magnetic kagome metals $R\mathrm{Mn_6Sn_6}$ (R = rare earth)

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Following the discovery of a quantum-limit magnetic Chern phase in $\mathrm{TbMn_6Sn_6}$ and the observations of a large topological Hall effect (THE) in the various field-induced magnetic phases in $\mathrm{YMn_6Sn_6}$ etc., the magnetic topological metals $R\mathrm{Mn_6Sn_6}$ (R = rare earth), that possess a bilayer kagome lattice of Mn, have recently emerged as a new platform to explore exotic quantum states that arise from the interplay between magnetism and non-trivial topological states in both *k*-space and real space. Understanding and eventual manipulation of these exotic quantum states can lead to potential technological applications in spintronics and quantum technologies. In this talk, I will mainly present our recent neutron scattering studies of static and dynamic magnetism in several representative magnetic topological metals $R\mathrm{Mn_6Sn_6}$, with the focus on possible temperature, magnetic-field, pressure and rare-earth tuning of their complex magnetism over a vastly different length scales, between colinear magnetic order, various zero-field and field-induced incommensurate spiral orders and possible non-coplanar spin textures. We have also observed a large THE that is directly associated with the field-induced non-coplanar incommensurate magnetic phase in these compounds. Our study has thus hinted a fascinating interplay between highly tunable magnetism and topologically non-trivial states in these bilayer kagome metals via intrinsic engineering of Berry curvature in both *k*-space and real space.

Novel Angular Anisotropy in Polarized Magnetic Small-Angle Neutron Scattering

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We report a hitherto unseen angular anisotropy in the polarized small-angle neutron scattering (SANS) cross section of a magnetically strongly inhomogeneous material. Based on a theoretical prediction, the normalized difference between the spin-up and spin-down SANS cross sections is expected to show a $\cos^2\theta$-type angular anisotropy. The effect is particularly pronounced in inhomogeneous magnetic materials such as nanoporous ferromagnets or nanocomposites, which exhibit large nanoscale jumps in the saturation magnetization at internal pore-matrix or particle-matrix interfaces. The present contribution addresses a fundamental question related to the angular anisotropy of the polarized SANS cross section. We discuss both result of the theoretical prediction as well as experimental results on a nanocrystalline inert-gas-condensed (IGC) Fe chosen as a demonstration system.

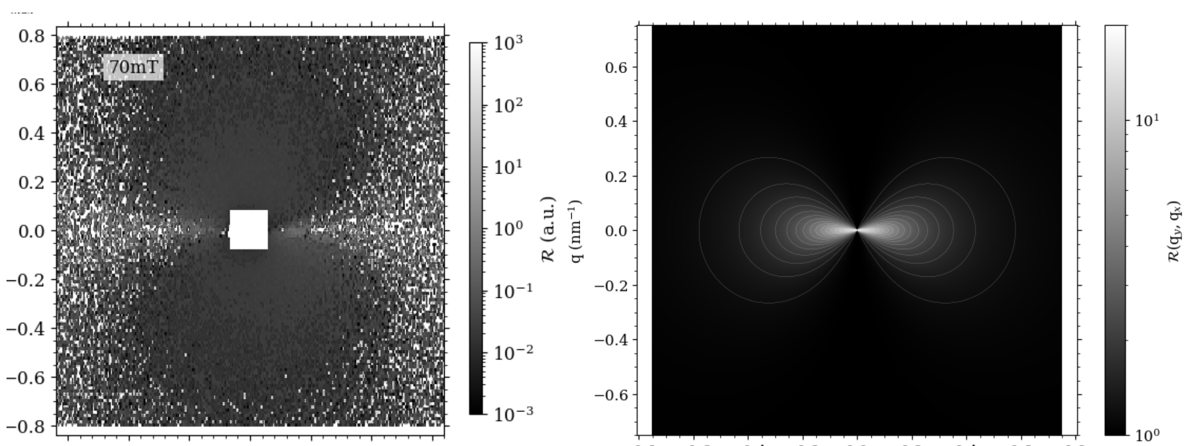

Fig. 1 Experimentally measured ratio (left) between the difference of the spin-up and spin-down SANS cross section of IGC Fe and theoretical prediction (left) of the normalized ratio for the same material parameters and fields.

Frustration vs. randomness in spin-1/2 triangular antiferromagnets

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Structural and quantum disorder in frustrated magnets can be intricately intertwined. I will illustrate their non-trivial relation using the example of $YbMgGaO_4$ that has been widely discussed as the spin-1/2 triangular spin-liquid candidate [1]. The formation of a spin liquid – an entangled spin state with exotic dynamics of fractionalized (spinon) excitations – is typically inferred from experimental signatures, such as the absence of local magnetic fields probed by muons and the excitation continuum witnessed by neutron scattering. While the aforementioned experimental probes affirm $YbMgGaO_4$ as a spin-liquid candidate, the actual physics of this material appears to be dominated by structural randomness. I will elucidate the mechanism of this randomness, its impact on the magnetic couplings, and the eventual ground state that can be understood as a random-singlet state with localized excitations involving valence bonds and orphan spins [2].

I will further show how the level of structural randomness can be reduced and eventually controlled in triangular antiferromagnets of the $AYbX_2$ family [3,4] (A = Na, K and X = O, S, Se), discuss prospects of stabilizing Dirac spin liquid and the dichotomy between 2D ordered and genuinely disordered states in triangular antiferromagnets.

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Neutron diffuse scattering, and disorder on the atomic scale

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The use of neutron diffuse scattering to study magnetic disorder on the atomic scale is currently riding on a wave of enthusiastic interest. The techniques are not new, dating from the first developments in neutron scattering methods, and were initially used primarily to study exotic magnetism in intermetallics, primarily spin glasses. These compounds have both crystallographic and magnetic short ranged order. Neutron scattering with polarization analysis is particularly powerful for these studies due to its ability to separate the nuclear and magnetic contributions to the diffuse scattering.

The current surge emerged in the late-2000s from the discovery of exotic physics in geometrically frustrated magnetic compounds, such as spin ice. The studied compounds have tended to be stoichiometric and hence tend not to have nuclear diffuse scattering. However, interest in the interplay between nuclear and magnetic short-ranged order is growing once again, with groups studying the effects solid solutions, reduced dimensionality, and defects and vacancies on the magnetic properties. Neutron scattering with polarization analysis will remain an essential technique for these studies.

I will strive to highlight some recent applications of neutron diffuse scattering with polarization analysis on magnetically frustrated compounds, summarizing the state-of-the-art in instrumentation world-wide and paying attention to developments of powerful data analysis techniques that provide unprecedented insight into the structure and dynamics.

Abstracts of Posters

(in alphabetical order)

Influence of randomness in 3D and 2D magnetic frustrated systems seen by neutron scattering

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In the search of experimental realizations for the spin-liquid state in frustrated magnets, the influence of structural disorder has often challenge the study of their properties as well as giving rise to unconventional magnetism [1-2]. In the frustrated triangular lattices described as the type $RABO_4$, the compound $YbMgGaO_4$ is a remarkable example, with an observed quantum spin liquid behavior that may be attributed to the disorder arising from the site mixing of Ga and Mg [3]. Investigations into its sister compound $YbZnGaO_4$ revealed a spin-glass ground state, attributed to the combined effects of chemical disorder and quantum fluctuation [4]. In this framework, we present neutron scattering studies in the fluorite compound $Dy_2Zr_2O_7$, which possesses an intrinsic disordered lattice. Here, the magnetic Dy^{3+} and the nonmagnetic Zr^{4+} cations occupy randomly a single indistinct site of a tetrahedral motif. Our neutron scattering studies detected no magnetic ordering even temperatures of only a few tens of millikelvins, and we observe a few thermodynamic similarities between $Dy_2Zr_2O_7$ and the pyrochlore spin ice $Dy_2Ti_2O_7$. However, spin-liquid characteristics instead of spin ice describe the character of the spin-spin correlations in $Dy_2Zr_2O_7$. Inelastic neutron scattering studies for the crystalline electric field (CEF) excitation down to 5 K show a broad and subtle energy spectre features. This remarks the strong effect of disorder, which modifies the ground state of Dy in the fluorite structure. In addition, I will introduce preliminary results of candidate materials for spin liquid, which are characterized by a triangular-layer-based lattice with non-disordered interlayers of transition metals nor intrinsic chemical disorder.

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Development of magnetic SANS at ISIS

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In this poster we will review the latest developments that have taken place in the SANS group at the ISIS neutron and muon source for investigations of magnetic materials, including sample environment like magnets, cryostats, furnaces and techniques like full polarisation analysis SANS.

Machine learning Based Data Analysis for Small Angle Neutron Scattering

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Small-angle neutron scattering (SANS) is one of the most important techniques for microstructure determination, which is utilized in a wide range of scientific disciplines such as materials science, physics, chemistry, and biology. Conventional SAS can probe microstructural (density and composition) inhomogeneities in the bulk and on a mesoscopic length scale between a few and a few hundred nanometers. Despite drastic improvements over the last decades, SANS is inherently flux limited, similar to any other neutron scattering technique, caused by the limited brilliance of todays neutron sources, that is essentially given by the target or core materials properties. Moreover, due to the large number of parameters and the lack of features in typical SANS data, SANS data analysis is often ambiguous and prone to overfitting and cognitive bias.

We show first results of an approach to automatize the analysis and fitting of SANS experiments. The machine learning algorithm has been trained using a large set of computer generated data of typical two-phase model samples with various shapes, concentrations and contrast, as a first step, independent of instrumental effects and instrumental resolution. Together with the AI based optimization of the measurement strategy, our project forms an important contribution to a fully autonomous SANS experiment.

Machine learning based Optimization of Measurement Strategies for Small Angle Neutron Scattering

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Small-angle neutron scattering (SANS) is one of the most important techniques for microstructure determination, which is utilized in a wide range of scientific disciplines such as materials science, physics, chemistry, and biology. Conventional SAS can probe microstructural (density and composition) inhomogeneities in the bulk and on a mesoscopic length scale between a few and a few hundred nanometers. Being sensitive to magnetism, small-angle neutron scattering (SANS) also provides a unique magnetic contrast. Despite drastic improvements over the last decades, SANS is inherently flux limited, similar to any other neutron scattering technique, caused by the limited brilliance of todays neutron sources, that is essentially given by the target or core materials properties.

We show first results of a recently popular approach to optimize the usage of SANS beamtime. In this project, we use algorithms based on machine learning to optimize and automatize the measurement strategy of a pinhole SANS instrument, based on a set of exemplary standard SANS samples. Our model includes the desired statistical resolution, intensity and Q-resolution for the different geometrical settings of the instrument and is able to provide reduced I(Q) data of a set of samples as an output. Together with the AI based fitting of the data, our project forms an important contribution to a fully autonomous SANS experiment.

References

Magnetic field dependent neutron diffraction studies of polycrystalline $Ho_3Fe_5O_{12}$

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The rare earth garnet system $Ho_3Fe_5O_{12}$ (HIG), which is ferrimagnetic below 567 K (T_C), shows a magnetization compensation phenomenon at 138 K (T_{Comp}), where the thermal difference of sublattice magnetizations reveals a complete cancellation of net magnetization [1]. In addition to magnetic compensation, single umbrella magnetic ordering of Ho^{3+} ion is observed with that of structural distortion (cubic to rhombohedral, Ia-3d to R-3) at T_{Comp}. Below the T_{Comp}, an interesting magnetic transition at ~50 K is observed with double umbrella ordering of Ho^{3+} ion moment due to the effect of crystal field energy. Also, the heat capacity measurements with an applied magnetic field across the T_{Comp} point out the significant influence of the external magnetic field on the evolution of umbrella orientation of Ho moments with a different angle. Therefore, to investigate the evolution of magnetic structure in the presence of an external magnetic field, we carried high resolution neutron diffraction experiments with applied magnetic fields up to 6T. We resolved the magnetic compensation with bipolar states of the magnetization reversal phenomenon with ordering of Ho moment.

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Magnetic order in the quasi-one-dimensional quantum magnet candidate compound $NdOCa_4(BO_3)_3$

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Low-dimensional magnetic materials have recently attracted much attention due to their diverse physics properties [1-2]. Quasi-1D quantum magnets can be found in 3d transition-metal oxide (TMO) systems, such as various copper oxide compounds [3-5]. Comparing to quasi-1D system in TMO, there are only very few investigations on the 4f rare-earth based compounds. NdOCa4(BO3)3 (NdCBO) shows a monoclinic crystal structure in which the nearest-neighbor (NN) distance between the rare-earth ions along the c axis is 3.8 A. On the other hand, the NN distance along the a/b direction is 8.3 A. It has recently been suggested that NdCBO system could be a good quasi-1D quantum magnet candidate compound.

Our DC magnetic susceptibility measurement on the single-crystal samples of NdCBO respectively along both x- and z-directions exhibit no indication of a long-range magnetic order transition can be seen down to 1.8 K in both orientations. Especially, the AC magnetic susceptibility measurements on this sample along same directions indicating the likely occurrence of a long-range magnetic order at T=0.75 K. In this report, we will present our recently detailed X-ray diffraction (XRD), neutron powder diffraction (NPD) studies as well as the in-house magnetic properties measurements on both the single-crystal and powder samples of NdCBO and give a comprehensive understanding the magnetic order in this system

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Tuning Atomistic Disorder in Nanoparticles

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Being intrinsic to nanoscale materials, defects and disorder have shown significant effects on the magnetic properties of nanoparticles, affecting both magnetization and spin disorder throughout the entire nanoparticle. For application in magnetic hyperthermia, a significant influence of structural and spin disorder on the magnetic heating efficiencies has been proposed [1].

Our long-term goal is to control the level and distribution of atomistic defects and the arising spin disorder in magnetic nanoparticles, with the aim to understand quantitatively the interrelation of structural disorder and magnetic heating efficiency. Magnetic SANS and diffuse scattering using polarized neutrons are versatile techniques to characterize the magnetic disorder on several length scales from nanoscale magnetic morphology and magnetization to atomistic spin disorder [2] and will hence be highly relevant for our study.

In this contribution, we will present our approach towards a careful synthesis design of ferrite nanoparticles, with the aim to influence the disorder of the crystal packing on the atomic level, and initial magnetic heating characterization.

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Spin order and disorder at interfaces in nanoscale magnets probed by neutron scattering

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Recent developments towards energy efficient devices have called for the development of strong permanent magnets based on rare earth elements. The atomic scale composition and spin order of the magnetic microstructure have a profound impact in developing the macroscopic magnetic information. The changes in magnetization occurring at nanoscale regime still needs to be addressed as the hysteresis of magnetic materials crucially depend upon the engineering of the microstructural and magnetic inhomogeneities including defects and the spin-order near the boundaries[1]. We would like to address these challenges through magnetic small-angle neutron scattering (SANS). SANS is a versatile technique to investigate chemical morphology and magnetization with nanoscale spatial resolution[2,3].

In this contribution, we will present our approach to the nanoscale magnetization in materials relevant for application as bulk ferromagnets. These will cover distinct microstructures, achieved through nanoscale precipitates by spinodal decomposition or during a tailored additive manufacturing process. Using magnetic SANS, we aim to extract parameters such as effective correlation length l_c of the spin misalignment within the microstructure which directly affects the desired macroscopic properties.

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The high-brilliance laboratory X-ray diffractometer GALAXI: from mesoscopic to interatomic length scales

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The high-brilliance laboratory (grazing incidence) small angle X-ray scattering instrument GALAXI [1] located at the Jülich Centre for Neutron Science allows investigations, at mesoscopic length scales, of chemical correlations in bulk materials or in assemblies deposited on a surface, and complements (grazing incidence) small angle neutron scattering studies. We will show some scientific results obtained at this instrument.

GALAXI is now being upgraded with a second 2D position sensitive detector and a cross cradle at sample position to perform (grazing incidence) wide angle X-ray scattering for the investigation of chemical correlations in the same systems as above, but at interatomic length scales. GALAXI will also be equipped with magnetic fields variable in direction and amplitude, using a setup based on a Halbach array of permanent magnets. We will detail those two projects.

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Bloch points in classical and quantum magnetic systems

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A Bloch point represents a three-dimensional hedgehog singularity of a magnetic vector field [Fig.1(a)] in which the magnetization vanishes. Experimentally, the appearance of such points is well-established; in particular, they can be hosted by magnetic bubbles and chiral bobbers or appear dynamically during the creation and annihilation of topologically non-trivial textures. At the same time, standard micromagnetic theory is developed for magnetic moments of a fixed length and is thus not completely applicable to the investigation of such singularities. To approach this problem, we study a Bloch point in a quantum Heisenberg model for the case of spin-1/2 particles. Such a state can be stabilized by adding a Zeeman term which mimics the hedgehog magnetization profile far away from the singularity. Performing an exact diagonalization of the Hamiltonian as well as using density matrix renormalization group techniques, we obtain the ground state, which can be used to recover the corresponding magnetization profile. Our findings demonstrate a variation of the spin length in the quantum model, leading smoothly to zero magnetization at the Bloch point [Fig.1(b)]. This behavior is generic for different system sizes. Our results indicate the necessity of generalizing the classical micromagnetic model by adding the third degree of freedom of the spins: the ability to change its length. I will discuss possible approaches to do this in my talk.

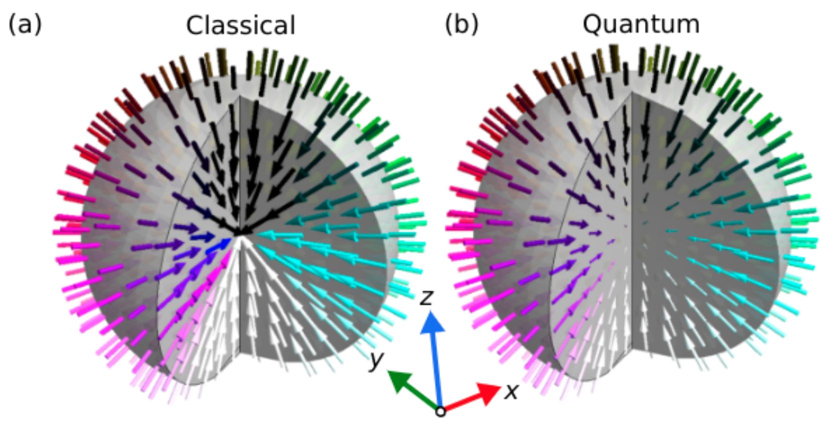

Figure 1. Magnetic textures of the quantum and classical Bloch points.

Signature of magnetic skyrmions in the chiral function

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We examine the chiral function in the polarized magnetic small-angle neutron scattering (SANS) cross section resulting from vortex-type and skyrmion spin structures through numerical micromagnetic simulations. Using the materials parameters of FeGe and adopting a cylinder geometry, we consider the interplay between the isotropic exchange interaction, the Dzyaloshinskii-Moriya interaction (DMI), a uniaxial magnetic anisotropy, a Zeeman energy, and the magnetodipolar interaction. We compare results with and without the DMI to understand its influence on the emergence of skyrmions and their signature in the chiral function. Our numerical computations are compared to an analytical trial field for the unit magnetization vector that is able to reproduce vortices as well as Bloch and Néel skyrmions. We show that, for the given system Hamiltonian and particle geometry, pure Néel skyrmions do not correspond to an energy minimum and yield a vanishing chiral function.

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Portable devices for extending resolution of small-angle neutron scattering instrument at FRM-II

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The magnetic Wollaston prisms (MWPs) are the devices used for manipulation of polarized neutron beams for the purpose of adding Spatial - Intensity - Modulation - mode (SIM-mode) to neutron scattering instruments.

One application for such devices is found in spin-echo small-angle (modulated) neutron scattering or SE(M)SANS [1]. There, MWPs allow extending the resolution of a typical SANS instrument from hundreds of nanometers to tens of micrometers, boosting the instrument's flexibility for different applications.

Another application of MWPs is found in combination with a resonant spin-echo technique, such as MIEZE technique implemented at the RESEDA instrument at the FRM II. The incorporation of MWPs into MIEZE instrument expands its originally limited to small scattering angles resolution to potentially any desired scattering angle [2]. In addition to that, the incorporation of SIM-mode devices to RESEDA would allow to use it as a SEMSANS instrument if required.

Finally, MWPs might be found useful in the context of intra-particle mode-entangled neutron beams for potential use in probing many-body quantum entanglement in materials [3].

In the present contribution, we provide an update on the construction progress of superconducting MWPs intended for use at FRM II, describe the details of their operation, and discuss the various possibilities they offer.

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Characterization of Magnetic Multilayers Deposited onto Nanosphere Arrays Using Grazing Incidence Small-Angle X-ray Scattering (GISAXS)

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Grazing Incidence Small-Angle X-ray Scattering (GISAXS) has emerged as a powerful tool for probing the structural properties of thin films and nanostructures with exceptional sensitivity and resolution. In this study, we employed GISAXS at GALAXI [1] to investigate the interplay between curvature and material properties in thin film systems. The morphology and ordering of $[Co/Pt]_n$ magnetic multilayers deposited using Molecular Beam Epitaxy (MBE) onto densely packed two-dimensional arrays of silica nanospheres with diameters of 50 nm and 200 nm, formed using an improved drop-casting method [2], will be presented. The deposition of thin films onto nanosphere arrays results in lateral variations in film thickness, which in turn gives rise to varying deposited material properties. The nanosphere arrays serve as an ideal template for the controlled growth and alignment of the magnetic layers, offering insights into the influence of curved surfaces on the resulting magnetic properties. By employing a rigorous analysis of GISAXS data in conjunction with complementary techniques such as magnetometry and microscopy, we are able to gain insight into the curvature-mediated modulation of structural and magnetic properties. Our findings contribute to the fundamental understanding of nanostructure-magnetic interactions and pave the way for the design of novel functional materials and devices tailored for applications in spintronics, magneto-optics, and magnetic recording.

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Magnetic microstructure of nanocrystalline Fe-Nb-B alloys as seen by small-angle neutron and X-ray scattering

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We have investigated the magnetic microstructure of two-phase Fe-Nb-B based Nanoperm alloys using unpolarized small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS). Our SANS analysis reveals a significantly large magnetic scattering contribution due to spin misalignment, primarily originating from the substantial jump in the longitudinal magnetization at the interfaces between the particles and the matrix. The magnetic scattering exhibits an angular anisotropy that resembles a clover-leaf-type pattern, consistent with the predictions of micromagnetic SANS theory. Analysis of the one-dimensional SANS data yields values for the exchange-stiffness constant and the average anisotropy and magnetostatic fields. The micromagnetic correlation lengths for all three samples are of similar magnitude and exhibit a field variation with sizes ranging between about 10-30 nm. We also find that the nuclear and magnetic residual scattering component of the SANS cross section exhibits a similar *q* dependency as the SAXS data. These findings further validate the applicability of micromagnetic SANS theory, and the mesoscopic information obtained is crucial for the advancement of the soft magnetic properties of this class of material.

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Spin Correlations in Assemblies of Iron Oxide Nanoparticles

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In recent decades, analyzing complex, disordered systems posed a challenging yet highly rewarding endeavor in the field of physics [1]. One intriguing area of investigation involves spin disorder [2], particularly in the context of magnetic nanoparticles. They exhibit a reduced saturation magnetization compared to their bulk counterparts that is the result of a substantial degree of spin disorder. Polarized SANS with longitudinal polarization analysis (POLARIS) is a powerful technique to distinguish between spin configurations in nanoscale materials [3]. Whereas correlated spin canting near the particle surface was revealed in arrangements of nanoparticles [4,5], non-correlated spin disorder has been reported throughout non-interacting nanoparticles [6,7]. These observations indicate that interparticle interactions might play a pivotal role for correlated spin canting.

In this contribution, we will present our work on the effect of decreasing interparticle distances, correlated with increasing dipolar interactions, on the magnetic morphology of iron oxide nanoparticles. By pyrolysis treatment of self-organized nanoparticle arrangements, a systematic increase of packing densities in nanoparticle assemblies was achieved and related to increased superparamagnetic blocking temperatures. We will present the results of a POLARIS experiment (D33/ILL) on the magnetic morphology of nanoparticles with varying interparticle interactions.

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Neutron scattering signature of the Dzyaloshinskii-Moriya interaction in nanoparticles

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The antisymmetric Dzyaloshinkii-Moriya interaction (DMI) arises in systems with broken inversion symmetry and strong spin-orbit coupling. In conjunction with the isotropic and symmetric exchange interaction, magnetic anisotropy, the dipolar interaction, and an externally applied magnetic field, the DMI supports and stabilizes the formation of various kinds of complex mesoscale magnetization configurations, such as helices, spin spirals, skyrmions, or hopfions. A question of importance in this context addresses the neutron-scattering signature of the DMI, in particular in nanoparticle assemblies, where the related magnetic scattering signal is diffuse in character and not of the single-crystal diffraction-peak-type, as it is e.g. seen in the B20 compounds. Using micromagnetic simulations we study the effect of the DMI in spherical FeGe nanoparticles on the *randomly-averaged* magnetic neutron scattering observables, more specifically on the spin-flip small-angle neutron scattering cross-section, the related chiral function, and the pair-distance distribution function. Within the studied parameter space for the particle size (60 nm $\leq L \leq$ 200 nm) and the applied magnetic field (-1 T $\leq \mu_0 H_0 \leq$ 1 T), we find that the chiral function is only nonzero when the DMI is taken into account in the simulations. This result is discussed within the context of the symmetry properties of the magnetization Fourier components and of the involved energies under space inversion. Finally, for small applied magnetic fields, we provide an easy-to-implement analytical correlation function for the DMI-induced spin modulations (with wave vector k_d). The corresponding randomly-averaged spin-flip SANS cross-section reproduces the main features found in the numerical simulations.

Bridging Experimental Insights and Theoretical Models to Decipher the Exchange Interactions in $CaCu_3Ti_4O_{12}$

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The perovskite-like compound, $CaCu_3Ti_4O_{12}$, with its unique dielectric properties, has primarily aimed to understand the mechanisms underpinning these properties, specifically focusing on its magnetism and the role of anisotropy in determining its magnetic structure. This study explicitly elucidates the exchange interaction and single-ion anisotropy in $CaCu_3Ti_4O_{12}$, integrating the outcome of magnetic structure and spin wave spectrum via neutron scattering technique. Besides, the theoretical model was enhanced by addressing the disputes existing in the assumption of second-order perturbation and by resolving the dd-excitation levels through resonant inelastic X-ray Scattering (RIXS).

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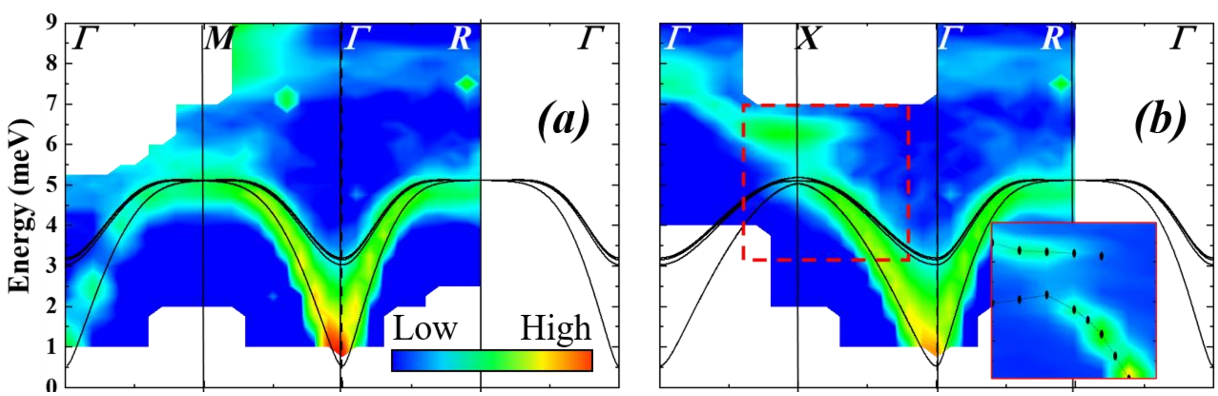

The magnon spectra measured at IN12 are contoured from the center of the Brillouin zone and along the (H,K,0), (H,H,L) and (H,H,H) reciprocal planes. The simulated magnon dispersions are depicted as black solid lines, and the corresponding high-symmetry positions, referenced to the simple cubic lattice, are marked on the top of the map.

The local structure of iron oxide nanoparticles upon lithiation

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Iron oxide nanoparticles are a promising alternative anode material for lithium-ion batteries due to their unique properties [1,2]. They offer high capacity, stability, and cost-effectiveness, addressing the demand for energy storage solutions. Iron oxide nanoparticles hold potential for next-gen energy storage technologies.

This study explores the local structural modifications occurring in iron oxide nanoparticles upon lithiation. We investigate the evolution of the local structure, including changes in crystallographic phases, lattice parameters, induced by lithium insertion. The findings provide insight into the mechanisms that underlie lithiation-induced structural transformations. This offers valuable information for the design an optimization new type of Li batteries.

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