“Trends in Quantum Magnetism” 2022
International Workshop

Book of Abstracts

Congressi Stefano Franscini,

Monte Verita,

24 – 27 April 2022

edited by
Kirill Povarov and Andrey Zheludev,
administrative assistance by
Alexandra Walby

April 23, 2022

The Workshop Program

Times: 08:00, 09:00, 10:00, 11:00, 12:00, 13:00, 14:00, 15:00, 16:00, 17:00, 18:00, 19:00, 20:00

Day 0 — April 24th
- Check-in
- Welcome drink
- Dinner

Day 1 — April 25th
- Welcome address
- **A**: Giamarchi; Honecker
- Coffee break
- **B**: Lake (online); Nayak; Masuda
- Lunch
- **C**: Petit; Tsvelik (online)
- Coffee break
- Group photo
- **D**: Spaldin; Hayashida; Starykh
- Poster session
- Dinner

Day 2 — April 26th
- **E**: Coldea; Valenti; Sibile
- Coffee break
- **F**: Chernyshev; Zaharko; Poree; Rønnow
- Lunch
- **G**: Perkins; Povarov; Broholm (online)
- Coffee break
- **H**: Batista (online); Zhitomirsky; Nikitin
- Trip to Brissago Island
- Conference Dinner

Day 3 — April 27th
- **I**: Shannon (online); Sakai (online)
- Coffee break
- **J**: Horvatić; Göhmann; Stern; Mila
- Lunch

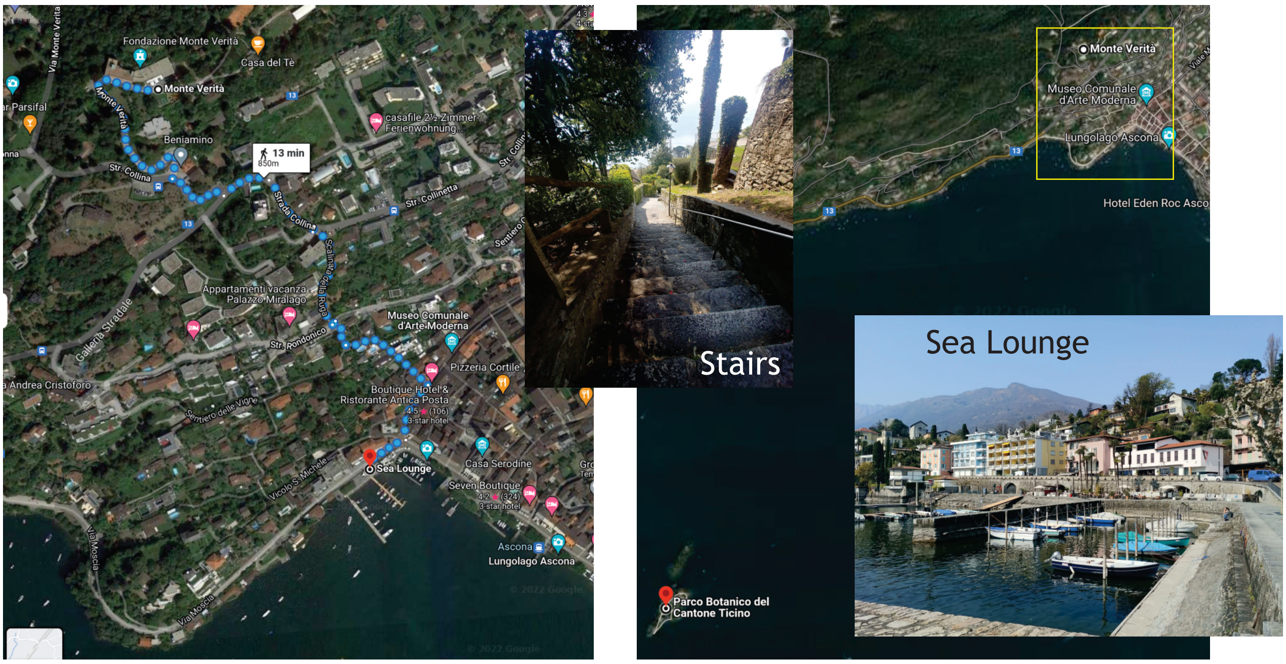
Information

About the Workshop

Quantum magnetism is a mature yet very active field of modern solid state physics, much boosted by F.D.M. Haldane's 2016 Nobel Prize. Recent breakthroughs in new materials synthesis, new experimental measurement techniques and new numerical methods have lead to a vast diversification of the field. Old standing puzzles got solved but many more complex problems suddenly appeared to be within our reach. Which directions of research are at the moment the most promising and exciting?

The aim of the "Trends in Quantum Magnetism" Workshop is to bring together the leading researchers from Switzerland and across the globe to promote an exchange of new results, new ideas and new challenges in both theory and experiment.

Conference Dinner



The Conference Dinner takes place on 26th of April on the Brissago Island. Our gathering point would be "Seven Sea Lounge" at the lakeshore, and the boat would take us from there at 18:00. The shortest walking route there from Monte Verita is about 10-15 min. However, it involves substantial amount of stairs. These can be avoided by taking an approximately twice longer route.

The boat would bring us to the island by 18:30, and the actual dinner would be preceded by an exciting excursion in the local botanical garden.

Day 0, 24 April 2022

Sunday is just the arrival day of the Workshop. The check-in in the Bauhaus hotel is possible after 15:00.

The Workshop opens

Welcome drink

Bar Roccia, 18:30

Dinner

Sala Luce, 19:00

Day 1, 25 April 2022

CSF welcome address

Auditorium, 09:00 — 09:15

Session A: 1D systems

Auditorium, 09:15 — 10:15

Chair: Mladen Horvatić

09:15 – 09:50

Quantum and topological transitions in the spin-chain compound $BaCo_2V_2O_8$

T. Giamarchi

University of Geneva

Quantum spin chains and ladders exhibit a host of properties quite different from their higher dimensional counterparts, including topological excitations such as spinons, and exotic physics such as the Tomonaga-Luttinger liquid. This physis has been spectacularly analyzed and observed in compounds such a BPCB or DIMPY.

I will discuss in this talk the physics of the compound $BaCo_2V_2O_8$, a spin chain compound, under magnetic field With a magnetic field transverse to the chain this compound allow to observe, by neutrons, a quantum phase transition between an Ising like phase and a flopped one with staggered magnetization perpendicular to the chains. Using both analytical and numerical studies we show that this transition is a topological one, characterized by a dual sine-Gordon field theory and study its properties [1,2]. When the field is longitudinal to the chain, another iconic transition occurs in this material: the Pokrovski-Talapov one between a commensurate magnetic phase and an incommensurate one [3]. In addition to discussing these transitions, I will present the difficulties both for this compound and numerous other, in taking properly into account the interchain (or interladder coupling) and discuss the resulting consequences for the phase diagram, as well as the theoretical challenges.

[1] Q. Faure, S. Takayoshi, S. Petit, V. Simonet, S. Raymond, L.-P. Regnault, M. Boehm, J. S. White, M. Månsson, Ch. Rüegg, P. Lejay, B. Canals, T. Lorenz, S. C. Furuya, T. Giamarchi, B. Grenier, Nature Physics **14**, 716 (2018).

[2] Q. Faure, S. Takayoshi, B. Grenier, S. Petit, S. Raymond, M. Boehm, P. Lejay, T. Giamarchi, V. Simonet, Phys. Rev. Research **3**, 043227 (2021).

[3] Q. Faure, S. Takayoshi, V. Simonet, B. Grenier, M. Månsson, J. S. White, G. S. Tucker, C. Rüegg, P. Lejay, T. Giamarchi, S. Petit, Phys. Rev. Lett. **123**, 027204 (2019).

09:50 – 10:08

Magnetothermal properties of the bimetallic ferromagnetically coupled chain compound $MnNi(NO_2)_4(en)_2$ (en = ethylenediamine)

Andreas Honecker[1], Maheshwor Tiwari[1], Wolfram Brenig[2], Ralf Feyerherm[3], and Stefan Süllow[4]

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[2]Institut für Theoretische Physik, TU Braunschweig, Germany

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Two energy scales are observed in the field-dependent specific heat of $MnNi(NO_2)_4(en)_2$ (en = ethylenediamine), containing ferromagnetically coupled chains with alternating spins of magnitude 1 and 5/2. $MnNi(NO_2)_4(en)_2$ orders antiferromagnetically at low temperatures in low magnetic fields, demonstrating relevant antiferromagnetic interchain coupling, with a suppression of this order already by a weak magnetic field. This strong effect of an applied magnetic field on the ordered state promises interesting magnetocaloric properties that we explore theoretically.

Specifically, we present numerical results for the specific heat obtained by exact diagonalization and Quantum-Monte-Carlo simulations for the alternating spin chain model, using parameters that have been derived from the high-temperature behavior of the magnetic susceptibility. The interchain coupling is included in the numerical treatment at the mean-field level. We also explore a simple single-site mean-field theory that is quantitatively less accurate, but more appropriate to describe the canted states in a magnetic field and thus the full phase diagram

Coffee break

Bar Roccia, 10:15

Session B: Exotic Excitations I

Auditorium, 10:45 — 12:15
Chair: Radu Coldea

10:45 – 11:20
Online talk

Excitations of the antiferromagnetic XXZ spin-1/2 spin chain - spinons, Bethe strings and E8 particles

B. Lake
Helmholtz Zentrum Berlin, Technical University Berlin

The antiferromagnetic spin-1/2 spin chain with Heisenberg-Ising (XXZ) anisotropy is a rich source of novel phenomena. Good physical realizations are $SrCo_2V_2O_8$ and $BaCo_2V_2O_8$ where the Co^{2+} ions have effective spin-1/2 and are coupled by antiferromagnetic interactions into chains while long-range magnetic order occurs at $T_N \approx 5$ K due to weak interchain coupling. The excitations are spinons which become bound into pairs below T_N. In a longitudinal field applied along the easy axis, the magnetic order is suppressed and using inelastic neutron scattering and optical spectroscopy we find the first evidence for complex bound states of magnetic excitations, known as Bethe strings [1,2], which were predicted almost a century ago [3]. Furthermore, the characteristic energy, scattering intensity and linewidth of the observed string states exhibit excellent agreement with precise Bethe-ansatz calculations. Application of a transverse field magnetic field perpendicular to the easy axis in $BaCo_2V_2O_8$ also yields interesting physics. At a field of $B = 4.7$ T we show that it realizes the quantum E8 integrable model, which is a massive relativistic quantum field theory containing eight gapped excitations characterized by the exceptional E8 Lie algebra [4,5].

[1] Z. Wang *et al.*, Nature **554**, 219 (2018)

[2] A. K. Bera *et al.*, Nature Physics **16**, 625 (2020)

[3] H. Bethe. Z. Phys. **71**, 205-226 (1931)

[4] H. Zou *et al.*, Phys. Rev. Lett. **127**, 077201 (2021).

[5] K. Puzniak *et al.* (to be published).

11:20 – 11:38

Magnetic-Field-Induced Bound States in Frustrated and Unfrustrated Spin-$\frac{1}{2}$ Ladders

Mithilesh Nayak[1], Dominic Blosser[2], Andrey Zheludev[2], Frédéric Mila[1]
[1]EPFL, [2]ETHZ

Motivated by the intriguing mode splittings in a magnetic field recently observed with inelastic neutron scattering in the spin ladder compound $(C_5H_{12}N)_2CuBr_4$ (BPCB) [1], we investigated the nature of the spin ladder excitations using density matrix renormalization group and simple analytical arguments [2]. We explore the dynamical structure factor of the frustrated ladder for different values of frustration, in which the bound states are observed close to $k = 0$ above first critical field (H_{c1}). We use the 2nd order perturbative expansion close to Fully Frustrated spin ladder to obtain the dispersion of bound states and these analytical conclusions match the numerical results perfectly. We numerically demonstrate the evolution of bound states as we decrease the frustration to reach the spin ladder case. The same analysis has been extended to higher energy bound states to provide a complete understanding of the features observed in the dynamical structure factor of the frustrated and the unfrustrated spin-ladder. The bound states are charac- terized by a field-independent binding energy and an intensity that grows with $H - H_{c1}$. These predictions are shown to explain quantitatively the split modes observed in BPCB.

[1] D. Blosser, V. K. Bhartiya, D. J. Voneshen, A. Zheludev, Phys. Rev. Lett. **121**, 247201 (2018)

[2] M. Nayak, D. Blosser, A. Zheludev, F. Mila, Phys. Rev. Lett. **124**, 087203 (2020)

11:38 – 12:13

Inelastic Neutron Scattering on Triagular Antiferromagnet $RbFeCl_3$ under Magnetic Field

S. Hasegawa[1], S. Asai[1], M. Matsumoto[2], T. Hong[3], B. Winn[3], T. Masuda[1]

[1]University of Tokyo, [2]Shizuoka University, [3]Oak Ridge National Laboratory

The investigation of materials that exhibit quantum phase transition provides valuable insights into fundamental problems in physics. Previously we presented neutron scattering under pressure in a triangular-lattice antiferromagnet $CsFeCl_3$ that has a quantum disorder in the low-pressure phase and a noncollinear structure in the high-pressure phase [1]. The neutron spectrum continuously evolved through critical pressure; a single mode in the disordered state became soft with the pressure and it splitted into gapless and gapped modes in the ordered phase. Extended spin-wave (ESW) theory revealed that the longitudinal and transverse fluctuations of spins were hybridized in the modes because of noncollinearity, and novel magnetic excitations were formed. This time we present neutron scattering under the magnetic field on an isostructural compound $RbFeCl_3$, of which the ground state is ordered near the quantum critical point. Evolution of the spectra with the magnetic field is successfully analyzed by ESW. Nontrivial behavior of the lifetime of magnon is discussed.

[1] S. Hayashida *et al.*, Sci. Adv. **5**, eaaw5639 (2019).

Lunch

Sala Luce, 12:30

Session C: Unusual degrees of freedom

Auditorium, 14:30 — 15:30

Chair: tbc

14:30 – 14:48

Spin dynamics and unconventional Coulomb phase in $Nd_2Zr_2O_7$

Mélanie Leger[1,2], Elsa Lhotel[1], Monica Ciomaga Hatnean[3], Jacques Ollivier[4], Andrew R. Wildes[4], Stephane Raymond[5], Eric Ressouche[5], Geetha Balakrishnan[3], Sylvain Petit[2]

[1]Institut Néel, CNRS and Université Grenoble Alpes, 38000 Grenoble, France

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[5]Université Grenoble Alpes, CEA, IRIG, MEM, MDN, 38000 Grenoble, France

Spin ice and more generally Coulomb phases are emergent states of matter that at- tract sustained attention in physics. Such systems lack long-range order, yet the ground state is formed, at the classical level, by degenerate configurations which satisfy a local organizing principle. In spin ice, this organization principle is known as the "ice rule" and states that each tetrahedron (building the pyrochlore structure of these materials) should have two spins pointing in and two spins pointing out. Even more fascinating, the ice rule can be interpreted as the divergence-free condition of an emergent fictitious magnetic field, while quantum fluctuations are expected to give rise to an emergent as- sociated electric field [1]. The route to stabilize such phases is to introduce transverse couplings, as opposed to Ising couplings at play in classical Coulomb phases. However, if too large, these transverse terms stabilize ordered phases. In this context, the question whether classical ordered phases may be stabilized out of Coulombic phase via a Higgs mechanism, also becomes an important issue. In this presentation, we tackle these questions experimentally in $Nd_2Zr_2O_7$ [2]. This pyrochlore magnet is indeed an excellent candidate: its ground state is antiferromagnetically ordered (all-in all-out AIAO state), but its paramagnetic phase above the ordering temperature remains enigmatic and could be a novel example of Coulomb phase [3]. High-resolution inelastic and polarized neu- tron scattering experiments especially draw a nice picture of the spin dynamics and of the magnetic correlations below and above the transition temperature ($T_N = 300$ mK), and confirm the coulombic nature of the phase above the ordering tem-perature, yet different from canonical spin ice.

[1] M. J. P. Gingras *et al.*, Rep. Prog. Phys. **77**, 056501, (2014)

[2] S. Petit *et al.*, Nature Phys. **12**, 746 (2016)

[3] M. Leger *et al.*, Phys. Rev. Lett. **126**, 247201 (2021)

[4] J. Xu *et al.*, Phys. Rev. Lett. **124**, 097203 (2020)

14:53 – 15:28
Online talk

Order Fractionalization in a Kitaev-Kondo model

A. Tsvelik
Brookhaven National Laboratory

We describe a mechanism for order fractionalization in a two-dimensional Kondo lattice model, in which electrons interact with a gapless spin liquid of Majorana fermions described by the Yao-Lee (YL) model. When the Kondo coupling to the conduction electrons exceeds a critical value, the model develops a superconducting instability into a state with charge e spinor order. By including an appropriate gauge string, we can explicitly show that spinorial order develops off-diagonal long range order.

Coffee break

Bar Roccia, 15:30

Group photo

In front of Bauhaus hotel, 16:00

Session D: Charge and quantum magnetism

Auditorium, 16:30 — 18:00

Chair: Roser Valenti

16:30 – 17:05

Hidden magnetoelectric multipoles

Nicola Spaldin
ETH Zürich

Most magnetic materials, phenomena and devices are well described in terms of magnetic dipoles of either spin or orbital origin. There is mounting evidence, however, that the existence and ordering of higher-order magnetic multipoles can lead to intriguing magnetic behaviors, which are often attributed to "hidden order" since they are difficult to characterize with conventional probes. In this talk I will discuss the relevance of the so-called magnetoelectric multipoles, which form the next-order term, after the magnetic dipole, in the multipolar expansion of the magnetization density in a magnetic field. First I will describe how magnetoelectric multipoles underlie multiferroic behavior and in particular how they determine the magnetic response to applied electric fields. Then I will discuss signatures of hidden magnetoelectric multipolar order, how it can be unearthed using density functional calculations and possibilities for its direct measurement. Finally, I will show that the bulk magnetoelectric multipolization manifests at surfaces as a magnetization, and explore an analogy with the bulk electric polarization and its associated surface charge.

17:05 – 17:23

Dielectric susceptibility at a magnetic BEC quantum critical point in $Rb_2Cu_2Mo_3O_{12}$

S. Hayashida
ETH Zürich

Bose-Einstein condensation (BEC) is the most celebrated of all phase transitions. Although a divergent susceptibility is one key property of any continuous phase transition, the critical susceptibility in BEC's original formulation is not physically accessible. This is because its order parameter is the complex amplitude of the condensate wave function. Hereby, we demonstrate that the critical susceptibility at a BEC quantum critical point can be measure directly through a dielectric channel in a multiferroic gapped magnet $Rb_2Cu_2Mo_3O_{12}$ [1]. Soft-mode ordering transition in gapped magnets can be described in terms of a BEC of magnons, where the order parameter, staggered magnetization, has a physical meaning. In $Rb_2Cu_2Mo_3O_{12}$, the typical BEC dome magnetic phase diagram is confined below 1.2 K [2], and the ferroelectric order emerges simultaneously with the field-induced magnetic transitions. Our dielectric measurements using single-crystal samples clearly demonstrates that the ferroelectric polarization is also a primary BEC order parameter [3]. The dielectric susceptibility is critical only at the upper quantum critical point not at the lower one. Notable finding is that the dielectric susceptibility at the upper quantum critical trajectory diverges as $1/T^{3/2}$. This behavior gives an excellent agreement with the theoretical prediction in 3D BEC quantum critical susceptibility.

[1] M. Hase *et al.*, Phys. Rev. B **70**, 104426 (2004)

[2] S. Hayashida *et al.*, Phys. Rev. B **100**, 134427 (2019)

[3] S. Hayashida *et al.*, Phys. Rev. Research **3**, 033053 (2021)[.5ex]

17:23 – 17:58

Electrical resistivity of the Kondo-like triangular lattice antiferromagnet in a magnetic field: the story of EuC_6

O. A. Starykh[1], A. L. Chernyshev[2]
[1]Department of Physics and Astronomy, University of Utah, USA,
[2]Department of Physics and Astronomy, University of California, Irvine, USA

Novel phenomena in magnetically-intercalated graphite has been a subject of much research in the 1980s. Among the most enigmatic findings of that era was a dramatic, roller-coaster-like behavior of the magnetoresistivity in EuC_6 compound [1], in which magnetic Eu^{2+} ions form a triangular lattice that is commensurate to graphite honeycomb planes. I present a microscopic explanation [2] of this behavior and demonstrate that the non-monotonic resistivity of EuC_6 is dominated by spin excitations in Eu-planes and their highly nontrivial evolution with the magnetic field. Our study highlights the crucial role of non-spin-flip electron-magnon scattering in the phases with non-collinear spin configurations as well as unusually strong sensitivity of the resistivity to the small biquadratic exchange interaction between localized magnetic moments. I conclude with comments on other synthetic two-dimensional magnets where electrical measurements can provide potentially significant insights into the nature of spin excitations.

[1] S. T. Chen *et al.*, Phys. Rev. B **34**, 423 (1986)

[2] A. L. Chernyshev, O. A. Starykh, Phys. Rev. X **12**, 021010 (2022)

Poster Session

Room Balint, 18:00 — 19:15

Exotic ordered phases in the distorted triangular quantum antiferromagnet Cs_2CoBr_4

L. Facheris[1], D. Nabi[1], K. Povarov[1], Z. Yan[1], E. Ressouche[2], D. Mazzone[3], S. Gvasaliya[1], A. Zheludev[1]

[1]Laboratory for Solid State Physics, ETH Zürich, 8093 Zürich, Switzerland

[2]Université Grenoble Alpes, CEA, IRIG, MEM, MDN, 38000 Grenoble, France

[3]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, 5232 Villigen, Switzerland

Single-crystal neutron scattering experiments and low-temperature thermodynamics revealed the competition of two frustration mechanisms in the 2D quantum antiferromagnet Cs_2CoBr_4. Key actors are the alternation of single-ion planar anisotropy direction of the individual magnetic Co^{2+} ions, and their arrangement in a distorted triangular lattice fashion. In particular, uniquely oriented Ising-type anisotropy emerges from the competition of easy-plane ones, and magnetic fields applied along this axis stabilize a cascade of five ordered phases. Among these, a field-induced incommensurate phase and an up-up-down plateau are found. Multiplexing inelastic neutron scattering is used to probe spin dynamics in zero-field and on top of the former state.

[1] K. Povarov, L. Facheris *et al.*, Phys. Rev. Res. **2**, 043384 (2020)

Hidden real-space and reciprocal-space magnetoelectric multipoles and their detection using Compton scattering

Sayantika Bhowal, Nicola A. Spaldin

Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, Switzerland

Magnetoelectric multipoles quantify the antisymmetric magnetization density of a solid in absence of both space-inversion $\mathcal{I}$ and time-reversal $\mathcal{T}$ symmetries. Such antisymmetric magnetization density of a magnetoelectric multipole is crucial to the understanding of the linear magnetoelectric response in a solid, that is, the linear order magnetization (electric polarization) induced by an applied electric (magnetic) field. Interestingly, a cross magneto-electric coupling can exist even in absence of any net electric polarization or magnetization, which makes the direct experimental detection of the magnetoelectric multipoles quite challenging with conventional probes. We show that due to the duality between real space and momentum space, the spin dependence of the magnetoelectric multipoles is very different in the reciprocal space from that of the real space, which can be used to design experiments for revealing these "hidden" orders. To be specific, the magnetoelectric multipole becomes an odd function of momentum k with no spin dependence in the reciprocal space, meaning that the antisymmetric magnetization density of a magnetoelectric multipole in the real space transforms into an antisymmetric electron momentum density. Since the real space-momentum space duality comes from the broken space inversion symmetry, an exactly opposite situation appears if we have an antisymmetric electron density (with no spin dependence) in the real space, e.g., in a ferroelectric system. In this case, the antisymmetric electron density in the real space transforms into an antisymmetric magnetization density which is an analogue of the magnetoelectric multipoles, albeit in the k-space. We show that the antisymmetric electron momentum density of a magnetoelectric multipole and the antisymmetric spin momentum density of its k-space analogues can be detected using designed Compton scattering [1,2] and magnetic Compton scattering [3] measurements respectively, providing a route to detect hidden magnetoelectric multipoles and their k-space analogues.

[1] S. Bhowal and N. A. Spaldin, Phys. Rev. Research **3**, 033185 (2021).

[2] S. Bhowal,D. O'Neill, M. Fechner, N. A. Spaldin, U. Staub, J. Duffy, and S. P. Collins, Open Research Europe **1**, 132 (2021).

[3] S. Bhowal, S. P. Collins and N. A. Spaldin, arXiv:2109.07315 [cond-mat.str-el] (2021).

Unconventional magnetoelectric coupling in highly frustrated one-dimensional spin systems

D. Flavián, S. Hayashida, Z. Yan, K. Yu. Povarov, S. Gvasaliya, A. Zheludev

Laboratory for Solid State Physics, ETH Zürich, 8093 Zürich, Switzerland

We report on the latest developments on the unique physics displayed by the frustrated quantum magnet $Rb_2Cu_2Mo_3O_{12}$ and $Cs_2Cu_2Mo_3O_{12}$. Much has been argued about the former magnetic and dielectric properties, including the existence of ferroelectricity driven by exotic spin-chiral order [1,2]. However, the lack of single-crystal samples was a patent problem, hampering further understanding of the underlying relevant mechanisms. We succeeded in growing macroscopic crystalline samples of both systems, which brought along a number of important breakthroughs [3,4]. Of particular interest are the results regarding the magnetic-field-tuned BEC of magnons. The measurable magneto- electric coupling in this material allowed to directly measure from the dielectric channel the critical susceptibility at a BEC transition, a quantity that is usually experimentally inaccessible or even nonphysical. The observed power-law behavior is in very good agreement with theoretical expectations for three-dimensional BEC [5]. Additionally, magnetic presaturation phases have been unveiled in this family of compounds, which may feature exotic order with unconventional broken symmetries.

[1] Y. Yasui, *et al.*, J. Appl. Phys. **113**, 17D910 (2013)

[2] H. Ueda, *et al.*, Phys. Rev. B **101**, 140408(R) (2020)

[3] S. Hayashida, *et al.*, Phys. Rev. B **100**, 134427 (2020)

[4] D. Flavián, *et al.*, Phys. Rev. B **101**, 224408 (2020)

[5] S. Hayashida, *et al.*, Phys. Rev. Research **3**, 033053 (2021)

Magnetoelectric multipole-based formalism for determining the surface magnetization of antiferromagnets

Sophie F. Weber, Nicola A. Spaldin

ETH Zürich, Switzerland

Antiferromagnets (AFMs) are ubiquitous in technological applications. They are essential components of the magnetic read heads in hard disk drives, in which they pin the magnetization of an adjacent ferromagnetic layer through exchange bias. Recently, they have also attracted interest as spintronic candidates due to their insensitivity to stray magnetic fields and their ultrafast spin dynamics.

A promising feature of AFMs with particular symmetries is the existence of an uncompensated magnetic moment per unit area at the surface of the AFM [1]. Indeed, for the case of magnetoelectric (ME) AFMs, the combined breaking of inversion and time reversal symmetries implies that there must exist surface terminations with uncompensated magnetization. The direction of this surface magnetization is directly connected to the underlying bulk domain, and can thus serve as a measurable probe. Moreover, uncompensated surface magnetization is thought to be the underlying cause of the above-mentioned exchange bias phenomenon, although the details are far from fully understood.

Recently, one of us proposed a convenient formalism for predicting the idealised, quantitative value of surface magnetization directly from a bulk quantity known as the magnetoelectric multipole tensor, $M_{ij} = \int r_i \mu_j(\mathbf{r}) d^3\mathbf{r}$ [2].

This tensor is required to be nonzero for a linear ME response to occur. Analogously to the bulk electric polarization, the ME multpole tensor is multivalued due to the periodicity of the lattice. However, once a particular surface direction and termination is selected, this fixes the "branch" of multipolization, and thus uniquely determines the multipolization tensor, and hence the uncompensated magnetization on this surface termination.

We first introduce the ME multipole-based formalization for predicting the surface magnetization of an AFM for a given surface direction and termination. We then apply the theory to the [001] surface of prototypical ME AFM, Cr_2O_3. Using Density Functional Theory calculations, we determine the electrostatically stable [001] termination, in agreement with experiment. The ME multipole tensor for this termination predicts an overestimated surface magnetization compared to results from recent experimental measurements on [001] Cr_2O_3 using nitrogen vacancy scanning magnetometry [3,4]. We reconcile this by showing with Monte Carlo simulations that the Cr magnetic moments at the [001] surface are likely disordered for temperatures well below the bulk Néel temperature. Recomputing the multipolization with the random orientation of surface spins taken into account, the theoretical prediction matches well with experimental estimates.

[1] K. D. Belaschenko, Phys. Rev. Lett. **105**, 147204 (2010)

[2] N. A. Spaldin, Journal of Experimental and Theoretical Physics **132**, 493-505 (2021)

[3] M. S. Wörnle *et al.*, Phys. Rev. B **103**, 094426 (2021)

[4] P. Appel *et al.*, Nano Lett. **19**, 1682 (2019)

Tuning the magnetic order in hexagonal manganites through zone-boundary structural modes

Tara N. Tošić[1], Quintin N. Meier[2] and Nicola A. Spaldin[1]

[1] ETHZ, [2]CEA Grenoble

Multiferroic hexagonal manganites (R-MnO_3) are prototype systems for studying highly frustrated magnetism due to their strong anti-ferromagnetic first nearest-neighbour coupling on a triangular lattice. The suppressed order is known to give rise to exotic phases such as spin liquids or extended critical regimes in this family of materials [1]. The exact magnetic order has been measured using second harmonic generation techniques [2], however the theory leading to a distinct magnetic symmetry is to date unclear. We propose that a planar triangular breathing mode (K_1) dictates the magnetic ground state. Using symmetry arguments, first-principles modelling and density functional theory, we describe in detail the magneto-structural coupling in this family of materials and explore small, and often ignored, ab-planar displacements of the magnetic sites that couple to the magnetic order. This work offers an answer to the on-going debate on the sub-Néel temperature displacements of the Mn sites and their importance in lifting the magnetic energy degeneracy in this frustrated system. By controlling structural changes within zone-boundary modes through external stimuli, modes such as K_1 could act as knobs that effectively tune the magnetic ground state. Furthermore, we open the discussion to a wider set of symmetry-allowed structural distortions that might have been overlooked in the past and could indeed be the result of important magneto-elastic effects, known to occur in the hexagonal manganites [3].

[1] S. Janas *et al.*, Phys. Rev. Lett. **126**, 107203 (2021)

[2] M. Fiebig *et al.*, Phys. Rev. Lett. **84**, 5620 (2000)

[3] S. Lee *et al.*, Nature **451**, 805 (2008)

Spin correlations in the frustrated ferro-antiferromanget $SrZnVO(PO_4)_2$

F. Landolt[1], K. Povarov[1], Z. Yan[1], S. Gvasaliya[1], E. Ressouche[2], S. Raymond[2], O. Garlea[3], K.M. Ranjith[4], M. Horvatić[4], and A. Zheludev[1]

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The layered vanadyl phosphates are hailed as proximate realizations of the ferro-antiferro-magnetic J_1-J_2 square lattice model which is suspected to host a nematic phase bellow saturation [1-3]. Indeed, bulk measurements on $SrZnVO(PO_4)_2$, a member of the vanadyl phosphates, have unveiled unusual presaturation behavior [4]. However, recently conducted NMR measurements provide clear evidence for a single-boson condensation at saturation, excluding a nematic presaturation phase [5]. This poster presents unpublished high field neutron diffraction data showing that the presaturation phase posses paramagnetic spin correlations. This findings make frustrated Dzyaloshinskii-Moriya interaction a plausible cause for the destabilization of the low field magnetic phase.

[1] N. Shannon, T. Momoi, and P. Sindzingre, Phys. Rev. Lett. **96**, 027213 (2006)

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[5] K. M. Ranjith, F. Landolt, S. Raymond, A. Zheludev, and M. Horvatić, to be published

Hidden magnetoelectric multipoles and their detection via neutron diffraction: the CuO case

Andrea Urru[1], Jian-Rui Soh[2], Navid Qureshi[3], Anne Stunault[3], Henrik M. Rønnow[2], and Nicola A. Spaldin[1]

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[2]Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

[3]Institut Laue-Langevin, 6 rue Jules Horowitz, BP 156, 38042 Grenoble Cedex 9, France

Magnetoelectric multipoles represent the first terms beyond the magnetic dipole moment in the expansion of a non-uniform magnetization density. They break both time-reversal and space-inversion symmetries, which ultimately links them to the magnetoelectric effect. In fact, any non-vanishing entry of the magnetoelectric tensor can be entailed by the presence of non-zero net magnetoelectric multipoles, and viceversa [1].

Magnetoelectric multipoles are often significantly smaller than the magnetic dipoles: as a consequence, the concurrent presence of a magnetic and, possibly, a magnetoelectric multipolar order makes their detection challenging. In this work we address the possible detection of multipolar hidden orders with neutron diffraction measurements. Neutrons interact with the full electronic magnetization density, however measurements are usually interpreted in the localized magnetic dipole moments picture. The theoretical formulation for the neutron scattering amplitude has been extended by S. W. Lovesey to include the contribution of the magnetoelectric toroidal moment [2]: in the present work, we review the theory and we further extend it to account for the magnetoelectric quadrupole moments as well.

As a relevant case of study, we consider CuO in the AF1 phase [3]. By means of *ab initio* techniques, we compute the magnetoelectric multipoles on both the Cu and O sites: we show that the presence of magnetoelectric toroidal and quadrupole moments can induce a difference between the xx and the yy (and zz) entries of the polarization matrix and we compare our predictions with spherical neutron polarimetry experimental results.

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[3] V. Scagnoli, U. Staub, Y. Bodenthin, R. A. de Souza, M. García-Fernández, M. Garganourakis, A. T. Boothroyd, D. Prabhakaran, and S. W. Lovesey, Science **332** (6030), 696-698 (2011).

Hydrodynamics of interacting spinons in the magnetized spin-1/2 chain with the uniform Dzyaloshinskii-Moriya interaction

Ren-Bo Wang[1], Anna Keselman[2], Oleg Starykh[1]

[1]Department of Physics and Astronomy, University of Utah, USA

[2]Physics Department, Technion, Haifa, Israel

We formulate an efficient hydrodynamic approach to obtain the dynamical spin susceptibility of an antiferromagnetic spin-1/2 chain with a uniform Dzyaloshinskii-Moriya (DM) interaction in presence of an external magnetic field. We find that transverse (with respect to the magnetic field) spin susceptibility harbors two (respectively, three) spin excitation modes when the magnetic field is parallel (respectively, orthogonal) to the DM axis. In all cases, the marginally irrelevant backscattering interaction between the spinons creates a finite energy splitting between optical branches of excitations at k=0. Our approximate analytical calculations compare well with numerical results obtained using matrix-product-state (MPS) techniques. Our findings are of immediate relevance to electron spin resonance experiments and other dynamic probes of the transverse spin susceptibility.

Anomalous spin waves in $S = 1$ triangular lattice antiferromagnets $CsFeCl_3$ and $RbFeCl_3$

L. Stoppel[1], S. Hayashida[1], Z. Yan[1], A. Podlesnyak[2], A. Zheludev[1]

[1]ETH Zürich, [2]Oak Ridge National Laboratory

The alkali-metal trichloroferrates AFeCl$_3$ ($A =$ Cs and Rb) are prototypical $S = 1$ triangular lattice antiferromagnets with strong easy-plane-type magnetic anisotropy [1]. Their ground states are a gapped singlet for $CsFeCl_3$ and a magnetically long-range ordered state for $RbFeCl_3$. Spin-wave excitations in both compounds have been extensively studied based on a model Hamiltonian with short-range interactions. At the same time, it is established that long-range magnetic dipolar interaction is relevant to the ground state in $RbFeCl_3$ [2]. However, the effect of magnetic dipolar interactions on the spin-wave excitation has not been investigated. To answer this question, we have carried out a detail analysis on the neutron scattering spectra by the extended spin-wave theory (ESWT) [3]. The analysis for $CsFeCl_3$ seems to work reasonably well but requires the introduction of additional exchange interactions. For $RbFeCl_3$, ESWT fails already on a quantitative level. The most remarkable result is that the observed spin-wave spectrum is highly anisotropic in the long-wavelength limit, whereas the ESWT simulation based on short-range interaction alone predicts an isotropic intensity. We conclude that this discrepancy is attributed to long-range magnetic dipolar interactions [4].

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[4] L. Stoppel *et al.*, Phys. Rev. B **104**, 094422 (2021)

Dinner

Sala Luce, 19:30

Day 2, 26 April 2022

Session E: Frustrated Systems I

Auditorium, 08:30 — 10:00
Chair: Alexander Chernyshev

08:30 – 09:05

Order-by-disorder in honeycomb $CoTiO_3$

Radu Coldea
Oxford University

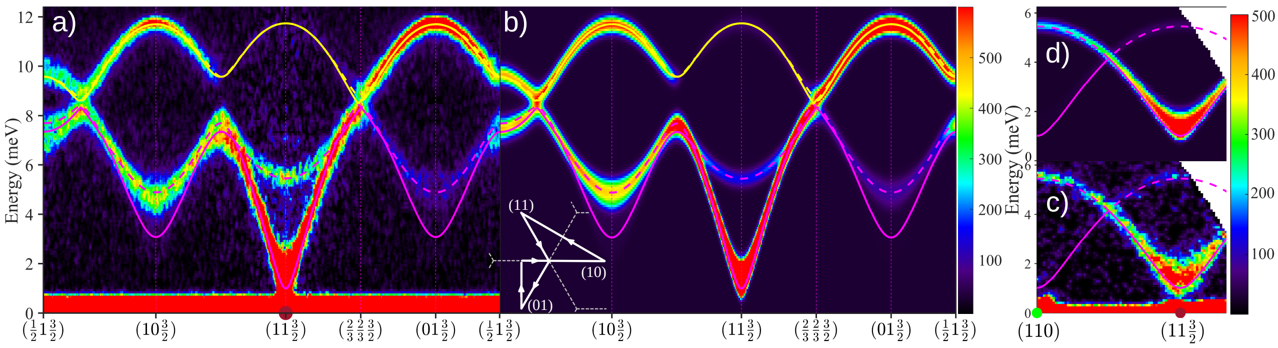

Figure 1: Magnon dispersions in $CoTiO_3$ along high-symmetry directions (a) in-plane and (c) out-of-plane, compared in (b) and (d) with a model calculation.

Order-by-disorder occurs when the ground state magnetic structure is selected out of a manifold of many classically-degenerate structures. We explore the manifestation of such physics experimentally in the honeycomb easy-plane magnet $CoTiO_3$ using high-resolution inelastic neutron scattering measurements of the magnetic excitations. We observe a finite energy gap above the magnetic Bragg peaks, which indicates a set of three symmetry-equivalent preferred moment directions in the ab plane. The gap cannot be understood classically considering only the lowest Kramers doublet (effective spin-1/2) of the Co^{2+} ions, as the mean-field energy is independent of the moment orientation in the ab plane for *any* two-site spin exchanges allowed by the rhombohedral crystal structure symmetry. As possible mechanisms for the gap generation we discuss i) zero-point quantum spin-wave fluctuations within the lowest Kramers doublet in the presence of bond-dependent exchanges and ii) spin-orbital exchange in the case when magnetic exchange, spin-orbit coupling and crystal field splittings are comparable as is the case here, and we provide a flavour-wave model to capture all key features of the observed spectrum [1].

[1] M. Elliot, P.A. McClarty, D. Prabhakaran, R.D. Johnson, H.C. Walker, P. Manuel and R. Coldea, Nature Communications **12**, 3936 (2021)

09:05 – 09:40

Electronic and magnetic properties of the RuX_3 (X=Cl, Br, I) family: Two siblings — and a cousin?

Roser Valenti
Institute of Theoretical Physics, Goethe University Frankfurt, Germany

Motivated by recent reports of metallic behavior in the newly synthesized RuI_3, in contrast to the Mott- insulating nature of the actively discussed α-$RuCl_3$, as well as $RuBr_3$, I will present a comparative analysis of the electronic and magnetic properties of this family of trihalides [1]. Using a combination of first-principles calculations and effective-model considerations, I will discuss that RuI_3, similarly to the other two members, is most probably on the verge of a Mott insulator, but with much smaller magnetic moments and a strong magnetic frustration. We predict the ideal pristine crystal of RuI_3 to have a nearly vanishing conventional nearest-neighbor Heisenberg interaction and to be a quantum spin liquid candidate of possibly different kind than the Kitaev spin liquid. In order to understand the apparent contradiction to the reported resistivity, I will present an analysis the experimental evidence for all three compounds and propose a scenario for the observed metallicity in existing samples of RuI_3. Furthermore, for the Mott insulator $RuBr_3$ I will introduce a magnetic Hamiltonian of a similar form to that in the much discussed α-$RuCl_3$ and show that this Hamiltonian is in agreement with experimental evidence in $RuBr_3$.

[1] David A. S. Kaib, Kira Riedl, Aleksandar Razpopov, Ying Li, Steffen Backes, Igor Mazin, and Roser Valenti, arXiv:2203.01626 [cond-mat.str-el]

09:40 – 09:58

Quantum spin ice states in cerium pyrochlores

R. Sibille[1], V. Porée[1], V. Pomjakushin[1], T. Fennell[1], N. Gauthier[2], E. Lhotel[3], S. Petit[4]
[1]Paul Scherrer Institut, [2]Sherbrooke University, [3]Institut Néel CNRS, [4]CEA

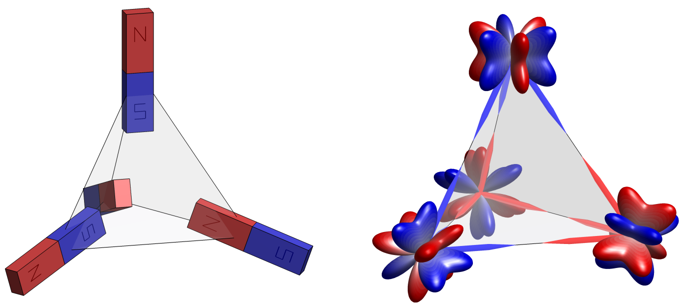

Figure 2: Spin ice and octupole ice configurations

A correlated liquid state was reported in the cerium stannate pyrochlore $Ce_2Sn_2O_7$ at temperatures below 1 Kelvin [1]. Its nature remained elusive, but with additional knowledge on the crystal-electric field scheme of cerium, recent works on $Ce_2Sn_2O_7$ [2] and $Ce_2Zr_2O_7$ [3-4] have further investigated the case based on degrees of freedom having both magnetic dipole and magnetic octupole components. Although these works vary in their details, they [2,4-6] remarkably agree towards a quantum spin ice (QSI) based on a manifold of ice-rule correlated octupoles (see figure). Earlier theoretical works [7-8] had conceptualised this octupolar QSI, where quantum dynamics is endowed by weaker couplings between other components of the pseudo-spins. The talk briefly reviews the findings reported so far on cerium pyrochlores [1-6], and additionally presents new experimental results that further hint at these materials being genuine representatives of a QSI – the model 3D quantum spin liquid.

[1] R. Sibille *et al.*, Phys. Rev. Lett. **115**, 097202 (2015)

[2] R. Sibille *et al.*, Nature Phys. **16**, 546-552 (2020)

[3] J. Gaudet *et al.*, Phys. Rev. Lett. **122**, 187201 (2019)

[4] B. Gao *et al.*, Nature Phys. **15**, 1052-1057 (2019)

[5] A. Bhardwaj *et al.*, arXiv:2108.01096 [cond-mat.str-el] (2021)

[6] E. M. Smith *et al.*, arXiv:2108.01217 [cond-mat.str-el] (2021)

[7] Y.-P. Huang, G. Chen, M. Hermele, Phys. Rev. Lett. **112**, 167203 (2014)

[8] Y.-D. Li, G. Chen, Phys. Rev. B **95**, 041106 (2017)

Coffee break

Bar Roccia, 10:00

Session F: Frustrated Systems II

Auditorium, 10:30 — 12:30

Chair: Oleg Starykh

10:30 – 11:05

Rethinking α-RuCl$_3$. Again

Alexander Chernyshev

University of California, Irvine

We argue that the available phenomenology significantly restricts the allowed model parameters for α-RuCl$_3$, a honeycomb-lattice magnet of great current interest, leading to its better understanding. It transpires that α-RuCl$_3$ can be described as an easy-plane ferromagnet with an antiferromagnetic further-neighbor and strong off-diagonal couplings. It is in a fluctuating zigzag ground state, which is proximate to an incommensurate phase that is neighboring a ferromagnetic one. We propose that the substantial anisotropic-exchange terms of the relevant models generically produce strong anharmonic couplings of magnons throughout the phase diagram and for any form of the underlying magnetic order, necessarily producing a spectrum of spin excitations that consists of a broad continuum coexisting with well-defined modes. For the much-discussed spectral properties of α-RuCl$_3$, the conclusion of this work thus unambiguously points toward the physics of strongly interacting and mutually decaying magnons, not to that of the fractionalized excitations.

*Funded by the DoE, Award No. DE-SC0021221

11:05 – 11:23

Magnetism in distorted Kagome-lattice intermetallic RAgGe family

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P. C. Canfield, S. L. Bud'ko

Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50010, USA

Kagome antiferromagnets are well-established model systems in theoretical condensed matter research. Experimental verification of theoretical solutions is, however, lagging as real systems obeying strict conditions of the ideal Kagome lattice are sparse. In the RAgGe family of compounds itinerant electrons enrich the problem of frustrated magnetism imposed by the distorted Kagome planes of the earth R+3 ions with strong magnetic easy-axis anisotropy. HoAgGe hosts a Kagome spin-ice [1]. YbAgGe reveals strong Kondo interaction and is located in a critical regime between long-range order of localised moments and non Fermi-liquid [2]. Metamagnet TmAgGe [3] possesses singu- larities of the Kagome Kondo-lattice model [4] in zero and applied magnetic fields. Here we present neutron scattering results for the R=Yb and Tm compounds [5, 6]. Theoretical envision of the experimental findings for this family of compounds is solicited.

Work in Villigen is supported by the Swiss National Science Foundation (Grant No. 200020-182536), work in Ames is supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering under Contract No. DE-AC02-07CH11358.

[1] K. Zhao *et al.*, Science **367**, 1218 (2020)

[2] Y. Tokiwa *et al.*, Phys. Rev. Lett. **111**, 116401 (2013) and references therein

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[5] C. Larsen *et al.*, Phys. Rev. B **104**, 054424 (2021)

[6] in preparation

11:23 – 11:41

Structural disorder and magnetic correlations in non-Kramers $Tb_2Hf_2O_7$ pyrochlore

V. Porée, P. M. Derlet, M. Kenzelmann, R. Sibille

Paul Scherrer Institut

The identification of possible mechanisms to stabilise Quantum Spin Liquid (QSL) phases [1] is of prime interest. In the case of non-Kramers pyrochlores, the introduction of transverse fields in the Hamiltonian was proposed theoretically [2-3], and argued experimentally [4], as a possible route to promote quantum fluctuations in spin ices [2-3].

Such physics was also proposed to be at work in $Tb_2Hf_2O_7$ [5], where experimental investigations have revealed the stabilisation of a spin liquid state despite a massive amount of disorder in the crystal, with about half of the terbium sites characterised by a defective coordination sphere. Here we present a detailed structural analysis of this material based on neutron pair distribution function (PDF) data, which we use to quantitatively relate to the magnetic properties.

We show how the big-box modelling of such a disordered material can be used to understand its crystal-electric field spectrum. The distribution of single-ion states, extracted from our model box including 2000 terbium sites, provides additional insights to explain the peculiar correlated magnetic ground state observed in $Tb_2Hf_2O_7$. We link these results with specific heat, ac-susceptibility, muon spin-relaxation and low-energy neutron spectroscopy data, allowing to further understand the partial spin freezing of about 15% of the sites occurring deep in the correlated phase. Our analysis indicates that this proportion of frozen degrees of freedom matches the number of doublets that are split by an energy scale exceeding that of the dominant interactions. More generally, we thus further demonstrate that for most of the spin system, where the doublet splitting is substantial but weaker than dominant interactions, pseudo-doublets are correlated to form a spin liquid.

[1] L. Balents, Nature **464**, 199 (2010)

[2] L. Savary and L. Balents, Phys. Rev. Lett. **118**, 087203 (2017)

[3] O. Benton, Phys. Rev. Lett. **121**, 037203 (2018)

[4] J.-J. Wen *et al.*, Phys. Rev. Lett. **118**, 107206 (2017)

[5] R. Sibille *et al.*, Nat. Commun. **8**, 892 (2017)

11:41 – 12:16

Quantum phases, transitions and excitations of $SrCu_2(BO_3)_2$

H. Rønnow

EPFL

Lunch

Sala Luce, 12:30

Session G: Exotic Excitations II

Auditorium, 14:00 — 15:30

Chair: Henrik Rønnow

14:00 – 14:35

Phonon dynamics in the Kitaev spin liquid

N. Perkins

University of Minnesota

The search for fractionalization in quantum spin liquids largely relies on their decoupling with the environment. However, the spin-lattice interaction is inevitable in a real setting. While the Majorana fermion evades a strong decay due to the gradient form of spin-lattice coupling, the study of the phonon dynamics may serve as an indirect probe of fractionalization in a quantum spin liquid. We show that the signatures of fractionalization of the Kitaev spin liquid into Majorana fermions and Z2 gauge fluxes can be seen in the sound attenuation, Hall viscosity and Fano shape of the Raman active optical phonons. We will discuss the implications of our findings to the candidate Kitaev materials.

14:35 – 14:53

Electron Spin Resonance as a Direct Probe of Spinon Interactions in $S = 1/2$ Chain

K. Yu. Povarov[1], T. A. Soldatov[2], R.-B. Wang[3], A. Zheludev[1], A. I. Smirnov[2], O. A. Starykh[3]

[1]Laboratory for Solid State Physics, ETH Zürich, 8093 Zürich, Switzerland

[2]P. L. Kapitza Institute for Physical Problems RAS, 119334 Moscow, Russia

[3]Department of Physics and Astronomy, University of Utah, Salt Lake City, Utah 84112, USA

The presence of strong, yet well-hidden backscattering between the fractionalized spinon excitations is known to be a part of the $S = 1/2$ chain physics for a long time. However, its dramatic consequences for the observable dynamical properties (such as the appearance of Fermi liquid's Silin mode analogue at small momenta) were realized only recently [1]. These details are challenging for observation, as they occur only in the magnetized state and only at nonzero momenta. We have succeeded in experimental detection of the associated dynamic features using Electron Spin Resonance as the probe [2]. This is only possible due to the specific "momentum boost" present in the spectrum of a unique spin chain material $K_2CuSO_4Br_2$ featuring the uniform Dzyaloshinskii–Moriya interaction pattern [3,4]. Description of the observed spectrum requires accounting for the backscattering even on the qualitative level. Quantitative analysis allows us to estimate the backscattering constant as $2.38J$. We also discuss the comparison between our results and the predictions of the Renormalization Group [5].

This work has been supported by the SNSF Division II (ETHZ), the National Science Foundation CMMT grant DMR-1928919 (U. Utah), and the Russian Science Foundation Grant 17-12-01505 (Kapitza Institute).

[1] A. Keselman, L. Balents, O. Starykh, Phys. Rev. Lett. **125**, 187201 (2020)

[2] K. Povarov, T. Soldatov, R.-B. Wang *et al.*, arXiv:2108.02835 (2021)

[3] M. Halg, W. Lorenz, K. Povarov *et al.*, Phys. Rev. B **90**, 174413 (2014)

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[5] S. Lukyanov, Nucl. Phys. B **522**, 533 (1998)

14:53 – 15:28
Online talk

Magnetic Excitations and Interactions in a Honeycomb Antiferromagnet

Collin Broholm[1], Thomas J. Halloran[1], Ruidan Zhong[2], and Robert J. Cava[3]

[1]John Hopkins University, [2]Shanghai Jiao Tong University, [3]Princeton University

$BaCo_2(AsO_4)_2$ is an effective spin-1/2 antiferromagnet that is of interest as a potential Kitaev spin liquid model system. At zero field there is incommensurate magnetic order for $T < 5.4$ K, which can be suppressed by an in-plane magnetic field of just 0.55 T. Here I report inelastic neutron scattering experiments probing the magnetic excitations. In the zero-field ordered state there are both resonant and continuous components to the spectrum with a minimal gap of 1.5 meV at $Q = 0$. For high in-plane field there are well-defined 2D ferromagnons from which we determine the magnetic interactions.

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331 and by the Gordon and Betty Moore foundation through the EPIQS program GBMF9456.

Coffee break

Bar Roccia, 15:30

Session H: Frustration, Order, and Disorder

Auditorium, 16:00 — 17:10
Chair: Natalia Perkins

16:00 – 16:35
Online talk

CP^2 Skyrmions and Skyrmion Crystals in Realistic Quantum Magnets

Hao Zhang[1], Zhentao Wang[2], David Dahlbom[1], Kipton Barros[3], and Cristian D. Batista[1]
[1]University of Tennessee, [2]University of Minnesota, [3]Los Alamos National Laboratory

Magnetic skyrmions are nanoscale topological textures that have been recently observed in different families of quantum magnets. These textures are known as CP^1 skyrmions because the target manifold of the magnetization field is the 2D sphere $S^2 \cong \mathrm{CP}^1$. We will demonstrate that magnetic CP^2 skyrmions can emerge in realistic spin-1 models. Unlike CP^1 skyrmions, CP^2 skyrmions can also arise as metastable textures of quantum paramagnets, opening a new road to discover emergent topological solitons in non-magnetic materials. The quantum phase diagram of the spin-1 models also includes magnetic field-induced CP^2 skyrmion crystals that can be detected with regular momentum (diffraction) and real-space (Lorentz transmission microscopy) experimental techniques.

16:35 – 16:53

Field induced order-disorder transition in easy-plane triangular antiferromagnet with defects

M. E. Zhitomirsky
IRIG, CEA-Grenoble

The nearest-neighbor triangular antiferromagnet is a paradigmatic model of magnetic frustration realized in many compounds. Notably, the 1/3 magnetization plateaus stabilized by quantum and thermal fluctuations via the order by disorder mechanism have been observed in $\mathrm{RbFe(MoO_4)_2}$, $\mathrm{Cs_2CuBr_4}$, and $\mathrm{Ba_3CoSb_2O_9}$. Impurities and bond defects can compete with the effect of fluctuations favoring the least collinear states and, thus, destroying the 1/3 plateau [1]. I will discuss a new spectacular effect caused by quenched disorder in easy-plane triangular antiferromagnets. Upon increasing in-pane magnetic field, the system undergoes a phase transition from an ordered state with the anti-Y spin configuration to a disordered high-field state. The high-field state lacks a long-range three-sublattice order. It consists of uncorrelated phase domains of the Imry-Ma type with sublattices reshuffled by defects. We give analytic and numerical arguments in support of such a phase transition at $T = 0$ for the XY triangular antiferromagnet. The recent magnetization measurements [2] find an evidence of such a transition in the model triangular antiferromagnet $\mathrm{Rb_{0.85}K_{0.15}Fe(MoO_4)_2}$, in which potassium doping induces random bond defects.

[1] V. S. Maryasin and M. E. Zhitomirsky, Phys. Rev. Lett. **111**, 247201 (2013)

[2] A. I. Smirnov et al., *Magnetization curve and phase diagram of triangular antiferromagnet RbFe(MoO4)2 with nonmagnetic substitution*, in press (2022)

16:53 – 17:11

Proximity to the Quantum-Spin-Liquid State in the Triangular-Lattice Antiferromagnet $\mathrm{CsYbSe_2}$

S. E. Nikitin[1], Tao Xie[2], S. Nishimoto[3], A. M. Läuchli[1,4], A. Podlesnyak[2]
[1]Paul Scherrer Institute, [2]Oak Ridge National Laboratory, [3]Technical University Dresden and IFW Dresden, [4]EPFL

The triangular-lattice antiferromagnet (TLAF) is one of the simplest geometrically frustrated models in condensed matter physics. The $S = 1/2$ TLAF with isotropic nearest-neighbour exchange interactions exhibits 120° order at zero temperature with reduced ordered moment. However, this state is relatively fragile, and weak perturbations, such as next-nearest-neighbour interactions or off-diagonal terms in the superexchange interaction, can stabilize new states such as quantum spin liquids (QSL) or stripe phases [1, 2].

In this presentation I summarize our recent results on the new perfect TLAF material $CsYbSe_2$ [3], which shows no transition into the long-range ordered state down to 0.02 K at zero field. However, we found that a Bragg peak with a relatively large in-plane correlation length is formed below approximately 0.4 K at the K point in the Brillouin zone, which is a fingerprint of a non-collinear 120° state. Application of a magnetic field suppresses this state and stabilizes the collinear $M/3$ plateau state in an intermediate field range of $B = 3 – 5$ T. The excitation spectrum evolves from strongly damped, continuum-like excitations at zero field to relatively sharp spin waves in the plateau phase. Above the plateau, the magnons again become strongly damped, before sharp spin waves reappear in the high-field regime, $B = 11$ T. Fitting of the high-field spectra with linear spin-wave theory yields a sizable next-nearest neighbour interaction, $J_2 = 0.05J_1$, which puts $CsYbSe_2$ very close to the boundary between the 120° and QSL phases [1]. To describe the spin dynamics over the whole field range we have employed large-cluster DMRG and ED calculations, and found good qualitative agreement between the calculate and measured spectra.

[1] Z. Zhu *et al.*,Phys. Rev. Lett. **120**, 207203 (2018)

[2] P. A. Maksimov *et al.* Phys. Rev. X **9**, 021017 (2019)

[3] T. Xie *et al.*, arXiv:2106.12451 [cond-mat.str-el] (2021)

Conference Dinner

- 17:55 Meeting near the Seven Sea Lounge
- 18:00 Boat travel to Brissago Island
- 18:30 Brissago Island Botanical Garden excursion
- 19:30 Dinner at Ristorante Isole de Brissago
- Boat travel back to Ascona

Day 3, 27 April 2022

Session I: Theoretical Advances

Auditorium, 09:00 — 10:00
Chair: Frederic Mila

09:00 – 09:35
Online talk

Semi-classical simulation of spin-1 magnets

N. Shannon
OIST

09:35 – 09:53
Online talk

Quantum spin nematic liquid of low-dimensional anisotropic magnets in magnetic field

Tôru Sakai
University of Hyogo and QST SPring-8

The spin nematic state [1,2] has attracted a lot of interest in the research field of the magnetism. It is the long-range quadrapole order of spins. It has bee theoretically predicted for various quantum spin systems, for example the bilinear-biquadratic models [3,4], the frustrated systems [5,6], etc. In most theories of the spin nematic behavior that have been proposed so far, the mechanism is based on the biquadratic interaction or the spin frustration. In this talk we propose simple theoretical models that exhibits the field-induced spin nematic liquid, without the biquadratic interaction or the frustration. They are the $S = 1/2$ spin ladder system with the anisotropic ferromagnetic exchange interaction, the $S = 1/2$ ferromagnetic-antiferromagnetic bond-alternating chain with the anisotropy, and the $S = 1$ antiferromagnetic chain with the single-ion anisotropy. In all the cases, the easy axis anisotropy plays a key role. In the previous work [7] the numerical diagonalization and the DMRG calculation indicated that the present model with the same amplitude between the antiferromagnetic leg and the ferromagnetic rung interactions gives rize to the field induced Tomonaga-Luttinger liquid phase where the quasiparticle is the two magnon bound state, as well as the $S = 1$ chain [8,9]. In the present work the critical exponent analysis indicates that the spin nematic correlation dominant region appears in the two-magnon Tomonaga-Luttinger liquid phase. In addition we present several phase diagrams with respect to the anisotropy and the magnetization. The magnetization curves calculated by DMRG are also presented for several typical cases [10].

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Coffee break

Bar Roccia, 10:00

Session J: Temperature Effects and Criticality

Auditorium, 10:30 — 12:30
Chair: Takatsugu Masuda

10:30 – 11:05

Critical low-energy spin dynamics in the BEC-type antiferromagnets

M. Horvatić
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The NMR nuclear spin-lattice relaxation rate (T_1^{-1}) data in spin systems provide privileged access to low-energy spin fluctuations, and are directly comparable to theoretical predictions for the corresponding spin-spin correlation functions. We address here T_1^{-1} data in the gapless and in the quantum critical regime of *unfrustrated* low-dimensional (D) quantum antiferromagnets, that is, above and in the vicinity of their magnetic-field-induced, low-temperature (T), 3D-ordered phase, described as the Bose-Einstein condensate (BEC). Our description is based on two seminal works [1] and provides their critical re-examination:

In particular, quasi-1D systems are addressed by the Tomonaga-Luttinger Liquid (TLL) theory, a purely 1D, effective, low-energy description, where the system is described by only two TLL parameters K and u that define respectively the power-law exponents of the response functions and the renormalized Fermi velocity. This provides a power-law prediction $T_{1TLL}^{-1} \propto T^{1/2K-1}$, corresponding to the zero-T criticality of a purely 1D system. However, the presence of the finite-T BEC transition at T_c provides a strong enhancement of spin fluctuations, extending high above T_c, recently described theoretically within the RPA approximation [2]. We show that this TLL+RPA description, which depends only on T_c and K, successfully describes $T_1^{-1}(T)$ data in two archetypal spin chains, and thereby enables a *direct* determination of the interaction parameter K [3].

The same description allows us to capture some effects of frustration and anisotropy, where the latter can provide an insight into quasi-2D systems, otherwise described only by advanced numerical simulations. As expected, preliminary experimental data on one quasi-2D system show stronger critical fluctuation than in 1D, suggesting that $T_1^{-1}(T)$ data could provide a clear signature for the system's effective dimensionality. However, here we have found only a partial agreement with the Quantum Monte Carlo (QMC) simulations, leaving the subject open to further investigation.

Finally, from a detailed study of the quantum critical (related to the saturation field) behaviour in the $SrZnVO(PO_4)_2$ compound [4], we learn that the predicted "critical" low-T limit $T_1^{-1} \propto T^{3/4}$ [1] is experimentally inaccessible, because: *i)* the convergence into this low-T limit is too slow, leading to unattainably low temperatures and *ii)* the theoretical prediction is no longer valid when the BEC transition is too close. Nevertheless, the complete description provides correct semi-quantitative account of the data.

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11:05 – 11:23

Thermal form factor series for the correlation functions of the Heisenberg-Ising chain

F. Göhmann
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The thermodynamic properties and finite temperature correlation functions of 1d quantum chains in the thermodynamic limit can be calculated within the quantum transfer matrix formalism. For the two-point functions of the Heisenberg-Ising chain we obtain so-called thermal form factor series [1] that are manifestly different from the form factor expansions with respect to the Hamiltonian basis. These novel series allow us to reconsider a number of longstanding problems. Examples considered so far include the high-T asymptotic analysis of the transverse two-point functions of the XX chain [2] as well as the two-point functions of spin-zero operators of the Heisenberg-Ising chain in the massive antiferromagnetic regime. For the latter we have obtained fully explicit and numerically highly efficient series representations for the longitudinal two-point functions [3] and for the correlation functions of two magnetic current densities that determine the dynamical conductivity.

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11:23 – 11:41

Absence of a dimensional reduction in the stable variant of $BaCuSi_2O_6$

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A prominent material where a two dimensional square lattice of dimers is realized and the appearance of a field-induced Bose-Einstein condensation (BEC) of triplons was reported, is $BaCuSi_2O_6$ [1]. The occurrence of magnetic field-induced ordered states, which can be described as BEC of triplons has the main idea behind that dimers of two Cu^{2+}-ions, which each carry a spin 1/2, can be mapped onto bosons to realize a BEC [2,3]. The interest in the compound as a material to observe a 3D-2D crossover at the quantum phase transition [4] vanished after the discovery of an incommensurately modulated low temperature structure with structurally inequivalent adjacent bilayers below 100K [5,6] complicating the model and its physics [7,8].
However, substitutions were reported to stabilize the tetragonal room temperature structure of $BaCuSi_2O_6$ down to lowest temperatures already with 5% Strontium substitution on the Barium place [8]. We present an analysis of the dimerized groundstate of $Ba_{0.9}Sr_{0.1}CuSi_2O_6$, the stable tetragonal structure variant of $BaCuSi_2O_6$. We explore the single particle excitation spectrum via inelastic neutron scattering and the high field groundstate with pulsed-field magnetization, specific heat, and magnetocaloric effect as well as static high field torque, and NMR studies. We find a single slightly broadened mode of single dimer kind in this "healed" structure. With the extracted interaction parameters we use Quantum Monte Carlo (QMC) calculations to describe our experimental phase border. Unlike proclaimed for $BaCuSi_2O_6$ we find a critical exponent of 0.69(9) and no dimensional reduction [9].

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11:41 – 12:16

Thermal properties of frustrated quantum magnets

F. Mila

Ecole Polytechnique Fédérale de Lausanne, Switzerland

The thermal properties of frustrated quantum magnets are a real challenge because, when formulated in the natural configuration basis, Quantum Monte Carlo simulations suffer from a very serious minus sign problem that excludes simulations below temperatures of the order of the coupling constants. In this talk, I will review recent numerical progress made on two fronts: (i) Quantum Monte Carlo simulations in the dimer basis [1]. In this basis, there is no minus sign problem for fully frustrated models, and simulations can be performed down to arbitrarily low temperature. With these simulations, we have identified the presence of a thermal critical point terminating a line of first-order transitions in the fully frustrated bilayer model [1]. (ii) Tensor network simulations [2,3]. Using ancilla spins and a partial trace, the thermal ensemble can be accurately obtained by imaginary time evolution, leading to reliable results down to temperatures only a few percents of the coupling constants regardless of the level of frustration. Using this approach, we have been able to show that the peak of the specific heat around 2 GPa and 4 K in $SrCu_2(BO_3)_2$ is a thermal critical point akin to that of the fully frustrated bilayer [2], and to numerically verify the long-standing prediction that the spin-1/2 J_1-J_2 model on the square lattice has a thermal Ising transition for large enough J_2/J_1 [3].

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Lunch

Sala Luce, 12:30

The Workshop closes