# International Conference on Highly Frusturated Magnetism 2018 University of California, Davis Conference Program





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# 0.1 Program at Glance

MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	SATURDAY
TUTORIAL I 9.00-12.00 Valenti, Taufour	Introductory remarks 8.30-9.00  PYROCHLORES I 9.00-10.30  Coldea, Gaulin, Jaubert	KITAEV I 8.30-10.00 Knolle, Halasz, Wu	KITAEV V 8.30-10.00 Matsuda, Motome, Lee	KAGOME I 8.30-10.00 Xiang, Kao, Fennell	FRUSTRATED MAG. III 8.30-10.00 Batista, Romhanyi, Tsvelik
	Coffee 10.30-11.00	Coffee 10.00-10.30	Coffee 10.00-10.30	Coffee 10.00-10.30	Coffee 10.00-10.30
	PYROCHLORES II 11.00-12.30 Rau, Castelnovo, Holdsworth	KITAEV II 10.30-12.00 Banerjee, Valenti, Kee	FRUSTRATED MAG. I 10.30-12.30 Rougemaille, Becca, Honecker, Poilblanc	KAGOME II 10.30-12.00 Lake, Reuther, Ralko	TRIANGULAR I 10.30-12.00 Chen, Mourigal, Chernyshev
Lunch 12.00-2.00	Lunch 12.30-2.00	Lunch 12.00-1.30	Lunch 12:30-1.30	Lunch 12:00-1:30	Lunch 12.00-1.30
TUTORIAL II 2.00-5.00 Savary, da Silva Neto	PYROCHLORES III 2.00-3.30 Shannon, Plumb, Benton	KITAEV III 1.30-3.00 Rousochatzakis, Kim, Ruiz		FRUSTRATED MAG. II 1.30-3.00 Broholm, Mendels, MacDougall	TRIANGULAR II 1.30-3.00 Starykh, Clark, Tanaka
	Poster I & Coffee 3.30-5.00	Poster II & Coffee 3.00-4.30	EXCURSION	Poster III & Coffee 3.00-4.30	Closing Remarks 3.00
	PYROCHLORES IV 5.00-6.30 Onoda,Petit, Kawamura	KITAEV IV 4.30-6.00 Pollmann, Udagawa, Shimizu		ITINERANT MAGNETS 4.30-6.00 Savary, Sibille, Lee	
	BANQUET 7.00-10.00	OXFORD Inst. Social 6.00-7.30			

## 0.2 Tutorials

NOTE: Tutorials are located at Peter A. Rock Hall (across the street from Student Community Center).

#### Monday, July 9 Tutorials

#### Morning session:

9.00 am - 10:00 am Roser Valenti
Frustrated Magnetic Materials from an ab initio perspective
10:00 am - 10:30 am Discussions
10:30 am - 11:30 am Valentin Taufour
How to grow a magnetic single crystal and then kill its magnetism
11:30 am - 12:00 noon Discussions

#### Lunch 12.00 pm-2.00 pm

#### **Afternoon session:**

2.00 pm - 3:00 pm Lucile Savary
Quantum Spin Liquids
3:00 pm - 3:30 pm Discussions
3:30 pm - 4:30 pm Eduardo da Silva Neto
Resonant x-ray scattering(RXS) for the study of spin, charge and lattice excitations
4:30 pm - 5:00 pm Discussions

0.2. TUTORIALS Page 3

# 0.3 Oral Program Schedule

#### Tuesday, July 10

Morning session: Pyrochlores I (Chair: Reinhard Kremer)

8.30 am - 8.45 am: S. Mani Tripathi, Professor of Physics and Associate Dean UC Davis

Welcome

8.45 am - 9.00 am: Ernie Glover, Gordon Moore Foundation

**EPIQS Program** 

9.00 am - 9.30 am: Radu Coldea (invited)

Quantum features in the spin dynamics of the frustrated pyrochlore Er<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>

9.30 am - 10.00 am: Bruce Gaulin

Short and long range ordered spin ice in the frustrated pyrochlore Tb<sub>2</sub>Ge<sub>2</sub>O<sub>7</sub>

10.00 am - 10.30 am: Ludovic Jaubert

Pyrochlore thin films

#### Coffee break 10.30 am - 11.00 am

#### Late morning session: Pyrochlores II (Chair: Reinhard Kremer)

11.00 am - 11.30 am: Jeffrey Rau (invited)

Anisotropic exchange in ytterbium magnets: breathing pyrochlores, spinels and beyond

11.30 am - 12.00 pm: Claudio Castelnovo

Dynamics of quasiparticle excitations in spin ice materials

12.00 pm - 12.30 pm: Peter Holdsworth

Multiple monopole phase transitions in spin ice

#### Lunch 12.30 pm - 2.00 pm

#### Afternoon session: Pyrochlores III (Chair: Jeffrey Quilliam)

2.00 pm - 2.30 pm: Nic Shannon Frustrating quantum spin ice 2.30 pm - 3.00 pm: Kemp Plumb

Continuum of magnetic excitations in the Heisenberg pyrochlore antiferromagnet NaCaNi<sub>2</sub>F<sub>7</sub>

3.00 pm - 3.30 pm: Owen Benton

Disorder and its consequences in Pr-based quantum spin ice

#### Coffee break

Poster session I: 3.30 pm - 5.00 pm

#### Evening session: Pyrochlores IV (Chair: Jeffery Quilliam)

5.00 pm - 5.30 pm: Shigeki Onoda

Magnetic monopoles in quantum spin ice under an electric field

5.30 pm - 6.00 pm: Sylvain Petit Dynamic quantum Kagome ice 6:00 pm - 6:30 pm: Hikaru Kawamura

Randomness-induced quantum spin liquid behavior in the s=1/2 Heisenberg antiferromagnet on the pyrochlore lattice

#### Wednesday, July 11

Morning session: Kitaev physics I (Chair: Natalia Perkins)

8.30 am - 9.00 am: Johannes Knolle (invited)

Dynamics of Kitaev spin liquids

9.00 am - 9.30 am: Gabor Halasz (invited)

Probing Kitaev spin liquids with resonant inelastic X-ray scattering

9.30 am -10.00 am: Liang Wu

Antiferromagnetic resonance and terahertz continuum in  $\alpha$ -RuCl<sub>3</sub>

#### Coffee break 10.00 am - 10.30 am

#### Late morning session: Kitaev physics II (Chair: Natalia Perkins)

10.30 am - 11.00 am: Arnab Banerjee (invited) Magnetic disorder, order and models of  $\alpha$ -RuCl<sub>3</sub> 11.00 am - 11.30 am: Roser Valenti (invited)

Field-induced phases in generalized Kitaev models and materials

11.30 am - 12.00 pm: Hae-Young Kee

Path to stable quantum spin liquids in spin-orbit coupled correlated materials

#### Lunch 12.00 pm - 1.30 pm

#### Afternoon session: Kitaev physics III (Chair: Andrzej Oles)

1.30 pm - 2.00 pm: Ioannis Rousochatzakis (invited) Quantum spin liquid in the semiclassical regime

2.00 pm - 2.30 pm: Yong-Baek Kim

Theory of a quantum spin liquid in hydrogen-intercalated honeycomb iridate, H<sub>3</sub>LiIr<sub>2</sub>O<sub>6</sub>

2.30 pm - 3.00 pm: Alejandro Ruiz

Hidden ferromagnetism in the Kitaev honeycomb iridates

#### Coffee break

Poster session II: 3.30 pm -5.00 pm

#### Evening session: Kitaev physics IV (Chair: Andrzej Oles)

5.00 pm - 5.30 pm: Frank Pollmann (invited)

Efficient simulation of the dynamics in frustrated spin systems

5.30 pm - 6.00 pm: Masafumi Udagawa Vison resonance in Kitaev spin liquids 6.00 pm - 6.30 pm: Yasuhiro Shimizu Quantum criticality of Kitaev spin liquid

#### Thursday, July 12

Morning session: Kitaev physics V (Chair: Michael Lawler)

8.30 am - 9.00 am: Yukitoshi Motome (invited) Majorana signatures in Kitaev quantum spin liquids

9.00 am - 9.30 am: Yuji Matsuda (invited)

Thermal Hall effect in a Kitaev spin liquid: A possible signature of Majorana chiral edge current

9.30 am - 10.00 am: Minhyea Lee

In-plane thermal conductivity study in 2D honeycomb lattice magnets

#### Coffee break 10.00 am - 10.30 am

#### Late morning session: Frustrated Magnetism I (Chair: Michael Lawler)

10.30 am - 11.00 am: Nicolas Rougemaille (invited)

Artificial spin systems as experimental simulators of frustrated magnets: from the fragmentation of magnetization to the

six vertex model

11.00 am - 11.30 am: Federico Becca

Dynamical structure factor of frustrated spin models: a variational Monte Carlo approach

11.30 am - 12.00 pm: Andreas Honecker

Quantum-Monte-Carlo approach to the thermodynamics of highly frustrated spin-1/2 antiferromagnets

12.00 pm - 12.30 pm: Didier Poilblanc

Search for topological SU(2) chiral spin liquids using iPEPS

#### Lunch 12.30 pm - 1.30 pm

Pick-up for Napa Trip 1.00 pm

#### Friday, July 13

Morning session: Kagome I (Mostly Kagome) (Chair: Frederic Mila)

8.30 am - 9.00 am: Tao Xiang (invited)

Gapless spin-liquid ground state in the spin-1/2 Kagome antiferromagnet

9.00 am - 9.30 am: Ying-Jer Kao

A two-dimensional classical spin liquid in quantum Kagome ice.

9.30 am - 10.00 am: Tom Fennell

Multiple Coulomb phase in the fluoride pyrochlore CsNiCrF<sub>6</sub>

#### Coffee break 10.00 am - 10.30 am

Late morning session: Kagome II (Chair: Frederic Mila)

10.30 am - 11.00 am: Bella Lake

Exploration of the quantum spin liquid state in Ca<sub>10</sub>Cr<sub>7</sub>O<sub>28</sub>.

11.00 am - 11.30 am: Johannes Reuther

A theory perspective on the spin liquid candidate material PbCuTe<sub>2</sub>O<sub>6</sub>

11.30 am - 12.00 pm: Arnaud Ralko

Importance of virtual singlets in RVB theory of quantum spin liquids

#### Lunch 12.00 pm - 1:30 pm

Afternoon session: Frustrated Magnetism II (Chair: Laura Heyderman)

1.30 pm - 2.00 pm: Collin Broholm (Invited)
Frustrated Magnetism in Pyrochlore Fluorides

2.00 pm - 2.30 pm: Philippe Mendels

Low- $T^{17}$ O NMR study of herbertsmithite crystals.

2.30 pm - 3.00 pm: Gregory MacDougall:

Pauling entropy and deviation from the dipole ice model in a spinel spin-ice candidate

#### Coffee break

Poster session III: 3.30 pm -5.00 pm

#### **Evening session: Itinerant Magnets** (Chair: Laura Heyderman)

5.00 pm - 5.30 pm: Lucile Savary (invited)

Singular angular magnetoresistance and spontaneous symmetry breaking in a magnetic nodal semimetal

5.30 pm - 6.00 pm: Romain Sibille (invited)

Investigations on quantum effects in some rare-earth pyrochlore oxides.

6.00 pm - 6.30 pm: SungBin Lee

Multipolar order and superconductivity in Pr(TM)<sub>2</sub>(Al,Zn)<sub>2</sub>0 Kondo Materials

## Saturday, July 14

Morning session: Frustrated Magnetism III (Chair: Sian Dutton)

8.30 am - 9.00 am: Cristian Batista (invited)

Dynamical structure factor of the triangular Heisenberg model

9.00 am - 9.30 am: Judit Romhányi (invited)

Topological bands and multipolar edge states in quantum magnets.

9.30 am - 10.00 am: Alexei Tsvelik

Chiral spin order in Kondo-Heisenberg systems

#### Coffee break

#### Late morning session: Triangular I (Chair: Sian Dutton)

10.30 am - 11.00 am: Gang Chen (invited)

Frustrated metal Pr<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> and spin liquid candidate YbMgGaO<sub>4</sub>

11.00 am - 11.30 am: Martin Mourigal (invited)

Anomalous spin dynamics in triangular quantum magnets

11.30 am - 12.00 pm: Sasha Chernyshev Topography and mimicry on a triangular lattice

#### Lunch 12.00 pm - 1.30 pm

#### Afternoon session: Triangular II (Chair: Lei Shu)

1.30 pm - 2.00 pm: Oleg Starykh

Spinon resonance of two-dimensional U(1) spin liquids with Fermi surfaces

2.00 pm - 2.30 pm: Lucy Clark

Two-dimensional spin liquid behaviour in the triangular-honeycomb antiferromagnet, TbInO<sub>3</sub>

2.30 pm -3.00 pm: Hidekazu Tanaka

Structure of magnetic excitations in a spin-1/2 triangular-lattice Heisenberg antiferromagnet Ba<sub>3</sub>CoSb<sub>2</sub>O<sub>9</sub>

#### **Closing of the conference:**

3.00 pm - 3.15 pm:

Singh/Wang

# 0.4 Pyrochlores I

Tuesday, 9-10:30 Coldea, Gaulin, Jaubert

#### Quantum features in the spin dynamics of the frustrated pyrochlore Er<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>.

R. Coldea (Oxford), P. McClarty (Max-Planck Institute, Dresden), J. Rau (Max-Planck Institute, Dresden), D. Prabhakaran (Oxford) and D. Voneshen (ISIS Pulsed Neutron Source UK)

The antiferromagnetic order in the frustrated pyrochlore magnet  $Er_2Ti_2O_7$  has been proposed to be selected by quantum fluctuations from a degenerate classical manifold [1-4]. Here we report high-resolution inelastic neutron scattering measurements of the spin dynamics in applied magnetic field to reveal, in addition to dominant one-magnon excitations, also significant multi-particle continuum excitations and magnon damping effects at high energies.

[1] L. Savary, K.A. Ross, B.D. Gaulin, J.P.C. Ruff, L. Balents, Phys. Rev. Lett. **109**, 167201 (2012). [2] M.E. Zhitomirsky, M. V. Gvozdikova, P.C.W. Holdsworth, R. Moessner, Phys. Rev. Lett. **109**, 077204 (2012). [3] K.A. Ross, Y. Qiu, J.R.D. Copley, H.A. Dabkowska, B.D. Gaulin Phys. Rev. Lett. **112**, 057201 (2014). [4] S. Petit, J. Robert, S. Guitteny, P. Bonville, C. Decorse, J. Ollivier, H. Mutka, M.J. P. Gingras, I. Mirebeau, Phys. Rev. B **90**, 060410(R) (2014).

#### Short and Long Range Ordered Spin Ice in the Frustrated Pyrochlore Tb<sub>2</sub>Ge<sub>2</sub>O<sub>7</sub>.

B.D. Gaulin (McMaster University), A.M. Hallas (McMaster University), J. Gaudet (McMaster University), C.R.C. Buhariwalla (McMaster University), M. Tachibana (NIMS Japan), N.P. Butch (NIST), S. Calder (Oak Ridge National Laboratory), M.B. Stone (Oak Ridge National Laboratory), C.R. Wiebe (University of Winnipeg), and G.M. Luke (McMaster University)

Low temperature heat capacity and neutron scattering measurements have been carried out on  ${\rm Tb_2Ge_2O_7}$ , a member of the cubic pyrochlore family  ${\rm Tb_2B_2O_7}$ , with  $B={\rm Ge}$ ,  ${\rm Ti}$ ,  ${\rm Sn}$ . The  $B={\rm Ti}$  member of this family,  ${\rm Tb_2Ti_2O_7}$ , displays a well-known, enigmatic disordered spin liquid state at low tempertures. Accordingly,  ${\rm Tb_2Ti_2O_7}$  has been proposed, among other possibilities, as a candidate for a quantum spin ice ground state. Our low temperature heat capacity measurements on  ${\rm Tb_2Ge_2O_7}$  show three distinct features: two broad humps at  $T_{\rm CEF}=6$  K and  $T^*=1.1$  K, and a sharp peak at  $T_C=0.25$  K, signifying a 1st order transition. Neutron diffraction measurements show that  ${\rm Tb_2Ge_2O_7}$  evolves into state with short-range  $\Gamma_9$  correlations. This is a "flattened" variant of the spin ice ground state occurring below  $T^*=1.1$  K, with  $\sim 1~\mu_B$  moments canted towards the local [110] directions. There is a strong upturn in the ordered moment and the correlation length below  $T_C=0.25$  K, signifying a transition to a long-range ordered state belonging to the  $\Gamma_9$  manifold, and possessing a net ferromagnetic moment along the [100] directions. Inelastic neutron scattering shows the formation of a weakly gapped magnetic spectrum at  $T^*=1.1$  K, and a larger gap, with concommittent decrease in inelastic intensity, below  $T_C=0.25$  K. These results are discussed in the context of short and long range ordered spin ice states, and are compared with the exotic ground states displayed by sister pyrochlore magnets  ${\rm Tb_2Ti_2O_7}[1,2]$  and  ${\rm Tb_2Sn_2O_7}[3]$ .

- [1]T. Taniguchi et al., Phys. Rev. B 87, 060408(R) (2013)
- [2]E. Kermarrec et al., Phys. Rev. B 92, 245114 (2015)
- [3]I. Mirebeau et al., Phys. Rev. Lett. 94, 246402 (2005)

#### Pyrochlore thin films.

L. Jaubert (CNRS), J. Rau (MPI-PkS), P. Holdsworth (ENS Lyon), M. Gingras (Waterloo)

Motivated by recent experimental realisations of pyrochlore thin films, we will explore in this talk some of the promising facets offered by the slab geometry. Thin films are a natural platform to study the confinement of spin-liquid gauge fields, the evolution from three to two dimensional spin textures and magnetic order. Depending on the type of substrate, interactions on orphan bonds on the surfaces can be varied away from their bulk values. This offers a tuning parameter for a new degree of frustration when spatial invariance is lost.

We will present in detail the consequences of open surfaces on the mechanism of order by disorder, taking  $Er_2Ti_2O_7$  films as a working example. The U(1) invariance of the  $Er_2Ti_2O_7$  ground state is known to be broken into  $Z_6$  by thermal and quantum fluctuations, favouring the so-called  $\psi_2$  states. In a pyrochlore slab grown along the [001] direction, this  $Z_6$  degeneracy is further broken into  $Z_2$  and  $Z_4$ , and the competing  $\psi_3$  states reappear. A complex competition between multiple orders take place, as a function of temperature and film thickness. A gradient of ordering spreads over long length scale inside the film while the nature of the phase transitions is blurred between two and three dimensional critical phenomena. Beyond the physics of films, this project also largely applies to surface effects in single crystals.

0.4. PYROCHLORES I

# 0.5 Pyrochlores II

Tuesday, 11-12:30 Rau, Castelnovo, Holdsworth

#### Anisotropic exchange in ytterbium magnets: breathing pyrochlores, spinels and beyond.

J. G. Rau (MPI-PKS), M. J. P. Gingras (Waterloo)

We consider the structure of anisotropic exchange interactions in ytterbium-based insulating rare-earth magnets built from edge-sharing octahedra. We argue the features of trivalent ytterbium and this structural configuration allow for a qualitative determination of the different anisotropic exchange regimes that may manifest in such compounds. The validity of such super-exchange calculations is tested through comparison to the well-characterized breathing pyrochlore compound  $Ba_3Yb_2Zn_5O_{11}$ . We then consider applications to three-dimensional pyrochlore spinels as well as two-dimensional honeycomb and triangular lattice systems built from such edge-sharing octahedra. We find an extended regime of robust, emergent weak anisotropy with dominant antiferromagnetic Heisenberg interactions as well as smaller regions with strong Kitaev and other anisotropies. We discuss the implications of our results for known compounds with the above structures, such as the spinels  $AYb_2X_4$  (A = Cd, Mg, X = S, Se), the triangular compound YbMgGaO<sub>4</sub>, which have recently emerged as promising candidates for observing unconventional magnetic phenomena. Finally, we speculate on implications for some unstudied honeycomb ytterbium magnets, as well as the possibility of unusual dynamics in the ytterbium spinels, as has been seen the  $Yb_2M_2O_7$  (M = Ti, Ge, Sn) pyrochlore compounds.

#### Dynamics of quasiparticle excitations in spin ice materials.

Claudio Castelnovo (University of Cambridge)

Some of the most exciting discoveries in strongly correlated systems in recent years are related to phases of matter that have a topological nature, often conveniently described as novel types of vacua that host emergent quasiparticle excitations. The quasiparticles and their underlying vacuum are heavily intertwined: the local correlations in the vacuum have an impact on the properties of the quasiparticles and, vice versa, the motion of the quasiparticles can change the nature of the underlying vacuum. Developing a theory based on this idea is generally a tall order, and the effects of such feedback mechanisms remain largely unexplored. In this talk we investigate this feedback mechanism in the context of spin ice materials. At the microscopic level, we argue that the spin dynamics originates from transvers components of the internal exchange and dipolar fields, and is characterised by two distinct spin flip rates determined by the surrounding spin configuration. This points at an entirely novel type of annealed dynamics in spin ice systems. The separation in rates can be remarkably large in quantum spin ice compounds. By studying the resulting spectral properties of the quasiparticle excitations, we are able to compute their contribution to the magnetic conductivity, in good agreement with experimental results.

#### Multiple monopole phase transitions in spin ice

P. C. W. Holdsworth (Ecole Normale Supérieure de Lyon), V. Raban (Ecole Normale Supérieure de Lyon), C. H. Suen (McMaster University) and L. Berthier (Université de Montpellier)

The dumbbell model of spin ice offers a rich phase diagram in the three dimensional space of parameters,  $\mu$ , the monopole chemical potential, T, the temperature and  $\Delta$ , a staggered chemical potential which breaks the  $Z_2$  symmetry of the diamond lattice, favouring monopole and double monopole crystallization.

The central mirror plane, with  $\Delta=0$  corresponds to the standard spin ice phase diagram within this approximation [1,2], with a transition from spin ice to "all-in-all-out" (AIAO) order that changes from first to second order via a multicritical point. A double winged structure emerges from this point, giving phase boundaries that terminate in continuous

lines of critical end points. The five phases are the Coulomb fluid (spin ice), two symmetry related fragmented monopole crystal phases [2,3], and the two double monopole crystal, AIAO phases. The critical end points are symmetry sustaining and in this sense liquid-gas like. The transition separating the monopole fluid and fragmented monopole crystal phase is a close cousin of that occurring in spin ice with a magnetic field placed along the [111] crystal field axis [4,5,6,7].

I will present results from simulation and mean field calculations inspired by the S=2 Blume-Capel model [8] that confirm this rich structure. The critical end point for  $\mu=-4.35$  K, (the value for  $Dy_2Ti_2O_7$ ) is studied in detail, for which we develop non-equilibrium dynamical scaling [7] and effective fluctuation-dissipation ratios.

Finally we note that in the spin ice material  $Ho_2Ir_2O_7$ , a  $\Delta$  is provided by the staggered internal magnetic field offered by the iridium ions, placing it in the fragmented crystal phase [9]. An accident of nature puts  $Ho_2Ir_2O_7$  far from the phase boundaries, but this work shows that by applying either physical or chemical pressure a whole family of new phase transitions is out there waiting to be observed.

#### REFERENCES.

- [1] R. G. Melko and M. J. P. Gingras, Journal of Physics: Condensed Matter 16, R1277 (2004).
- [2] M. E. Brooks-Bartlett, S. T. Banks, L. D. C. Jaubert, A. Harman-Clarke, and P. C. W. Holdsworth, Phys. Rev. X 4, 011007 (2014).
  - [3] R. A. Borzi, D. Slobinsky, and S. A. Grigera, Phys. Rev. Lett. 111, 147204 (2013).
  - [4] R. Higashinaka, H. Fukazawa, K. Deguchi, and Y. Maeno, J. Phys. Soc.(Japan) 73, 2845 (2004).
  - [5] H. Aoki, T. Sakakibara, K. Matsuhira, and Z. Hiroi, J. Phys. Soc. (Japan), 73, 2851 (2004),
  - [6] C. Castelnovo, R. Moessner, and S. L. Sondhi, Nature 451, 42 (2008).
  - [7] J. Hamp, A. Chandran, R. Moessner, and C. Castelnovo, Phys. Rev. B 92, 075142 (2015).
  - [8] D. Pena Lara and J. A. Plascak, J. Mod. Phys. B, 12, 2045, (1998).
  - [9] E. Lefrancois, et. al., Nature Communications 8, 209 (2017).

# 0.6 Pyrochlores III

Tuesday, 2-3:30 Shannon, Plumb, Benton

#### Frustrating Quantum Spin Ice

N. Shannon (OIST), O. Benton (RIKEN), L. Jaubert (CNRS), M. Taillefumier (ETH), J. Oitmaa (UNSW), R. Singh (UC Davis)

"Quantum spin ice" materials have been widely discussed in terms of an XXZ model on a pyrochlore lattice. For unfrustrated interactions,  $J_{\pm}>0$ , this model is accessible to quantum Monte Carlo simulation and plays host to a celebrated example of a U(1) quantum spin liquid (QSL). These results have generated considerable excitement, not least because of the tantalising possibility of making a direct comparison with experiment. However there is no *a prioiri* reason to expect a quantum spin ice material to posses unfrustrated interactions, with explicit calculations for Pr-based pyrochlores predicting  $J_{\pm}<0$  [1]. And at present, relatively little is known about what should happen in this case [2].

In this talk we argue that the properties of a quantum spin ice may become even more interesting once it is "frustrated". Using a broad range of analytic and numerical techniques, we explore the new phases which arise in the XXZ model on the pyrochlore lattice for  $J_{\pm} < 0$ . At finite temperature, we find that the frustrated model supports not one, but three distinct forms of spin liquid: the easy-axis spin liquid spin ice; a  $U(1)\times U(1)\times U(1)$  spin-liquid governed by a point with SU(2) symmetry; and an entirely new form of easy-plane spin liquid described by a  $U(1)\times U(1)$  gauge group. We present explicit predictions for inelastic neutron scattering in each of these cases [3]. Meanwhile, in the quantum limit, for T=0, we find that spin ice gives way to the expected U(1) QSL in its  $\pi$ -flux phase [2], while the easy-plane spin liquid transforms into a nematic QSL. We provide a variational argument which shows how these two different phases are connected at the SU(2) point [4].

These results offer a rare opportunity to explore how one spin liquid transforms into another, and suggest that experimental studies of pyrochlore magnets may still have a great many more surprises in store.

REFERENCES. [1] S. Onoda and Y. Tanaka, Phys. Rev. B 83, 094411 (2011); [2] S. B. Lee, S. Onoda, and L. Balents, Phys. Rev. B 86, 104412 (2012); [3] M. Taillefumier, O. Benton, L. Jaubert, N. Shannon, Phys. Rev. X 7, 041057 (2017); [4] O. Benton, L. Jaubert, R. Singh, J. Oitmaa, N. Shannon, preprint.

#### Continuum of magnetic excitations in the Heisenberg Pyrochlore Antiferromagnet NaCaNi<sub>2</sub>F<sub>7</sub>

K. Plumb (Brown University), H. Changlani (Johns Hopkins University), A. Scheie (Johns Hopkins University), S. Zhang (Johns Hopkins University), J. Krizan (Princeton University), J. Rodriguez-Rivera (NIST Center for Neutron Research), Y. Qiu (NIST Center for Neutron Research), R. Cava (Princeton University), C. Broholm (Johns Hopkins University)

While the existence of a spin-liquid for Heisenberg spins on the pyrochlore lattice was first speculated by Jacques Villain nearly 40 years ago, there have been no controlled experimental realizations — either classical or quantum — of this model. In real materials, the putative spin-liquid is more often than not preempted by small perturbations or intrinsic disorder that stabilize a broken symmetry state. In this talk, I will discuss a new material, NaCaNi<sub>2</sub>F<sub>7</sub>, which realizes the isotropic spin liquid of Villain but with the additional complication of random Na<sup>+</sup> - Ca<sup>2+</sup> charge disorder in the crystal structure. Neutron scattering and calorimetric measurements were used to uncover the magnetic correlations in this material and fully determine the magnetic Hamiltonian. The ionic disorder creates a rugged energy landscape that acts to freeze a small fraction of the magnetic degrees of freedom in time. However, the energy scale set by this disorder is small, and the Heisenberg interactions prevail. In fact, only 40% of the available moment is frozen, and the magnetism in NaCaNi<sub>2</sub>F<sub>7</sub> is dominated by a persistently fluctuating component. These measurements provide the first experimental confirmation of Villain's prediction and a new insight into the interplay between disorder and magnetic exchange interactions in highly frustrated magnets.

#### Disorder and its consequences in Pr-based quantum spin ices.

Owen Benton (RIKEN Center for Emergent Matter Science)

Pr-based pyrochlores, such as  $Pr_2Zr_2O_7$  and  $Pr_2Hf_2O_7$ , have emerged as promising candidates for the realization of a quantum spin liquid ground state. Interest in these materials is fuelled not only by a lack of conventional magnetic order, but also by neutron scattering measurements tantalisingly reminiscent of predictions for a U(1) spin liquid [1,2]. Recent work has highlighted how quenched structural disorder plays a crucial role in these systems, by splitting the low lying crystal electric field doublets [3,4,5]. Here, I present a theoretical treatment of these effects, deriving a phase diagram for disordered Pr pyrochlores based on a controlled perturbation theory. This perturbation theory allows us to address the two key instabilities of the spin liquid phase—spinon condensation and confinement—in a quantitative way. Calculating the thresholds for each kind of instability allows us to infer a phase diagram for Pr pyrochlores in the presence of quenched structural disorder.

By comparing published thermodynamic data to numerical linked cluster calculations, we are able to quantify the strength of disorder in currently studied Pr pyrochlores, and thus to locate them on the phase diagram. This study resolves some long-standing mysteries about these materials and has implications for the prospects of realising a spin liquid ground state in experiment [6].

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# 0.7 Pyrochlores IV

Tuesday, 5-7 Onoda, Petit, Kawamura

#### Magnetic monopoles in quantum spin ice under an electric field.

S. Onoda (RIKEN) and S, Nakosai (RIKEN)

Unambiguously generating and detecting magnetic monopole current in quantum spin ice have been intriguing issues in frustrated magnets. The dconfined bosonic U(1) quantum spin liquid phase hosts magnetic monopoles as quasiparticles fractionalized from spins. In principle, magnetic monopoles may be directly detectable, for instance, through thermal transport phenomena. However, it remains open to discriminate the magnetic monopole contribution to heat current from the others. Here, we demonstrate theoretically two nontrivial phenomena of deconfined magnetic monopoles in quantum spin ice. Both are based on an observation that the symmetry requires a coupling between an external electric field/polarization and a fictitious electric gauge flux directly transmitted to magnetic monopoles [1]. Firstly, we show that an electric field applied to the edges of the U(1) quantum spin liquid creates the fictitious electric gauge flux for deconfined magnetic monopoles in the bulk and bends their orbital motion. This leads to antisymmetric tensor components in transport coefficients of magnetic monopoles and thus a heat carried by them [2], in an analogy to Hall transport phenomena of electrically charged particles under a magnetic field or with a uniform magnetization [3]. Secondly, we show that dissipationless magnetic monopole supercurrent can be generated across a tunnel junction of, for instance, two charge-1 Higgs confined ferromagnets weakly linked through the U(1) quantum spin liquid under an applied electric field parallel to the interface [1]. Finally, we discuss possible experimental setups for the two phenomena using candidate materials  $Pr_2Zr_2O_7$  and Propose a way of directly and unambiguously detecting magnetic monopole current.

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#### Dynamic quantum kagome ice.

S. Petit (Laboratoire Léon Brillouin, France), E. Lhotel (Institut Néel, France), M. Ciomaga Hatnean (University of Warwick, United Kingdom), J. Ollivier(Institut Laue Langevin, France), H. Mutka (Institut Laue Langevin, France), E. Ressouche (CEA Grenoble, France), M. R. Lees (University of Warwick, United Kingdom), G. Balakrishnan (University of Warwick, United Kingdom)

In spin ice physics, although different at first glance, the pyrochlore and kagome lattices are intimately related. Indeed, applying a magnetic field along the [111] direction of the pyrochlore structure allows the freezing out of the apical spins, and establishes a connection with the two dimensional physical characteristics of the kagome lattice. Provided the field is not too large, a degeneracy persists within the kagome planes: the 2 in --2 out ice rule transforms into the kagome ice rule, with 2 spins pointing into each triangle, and 1 out, or vice versa [1]. In this context, we report here a study of the effect of a [111] field on the ground state of  $Nd_2Zr_2O_7$ . In this pyrochlore magnet, classical spin ice physics is considerably modified by the existence of transverse terms in the Hamiltonian: spin ice signatures are transferred in the excitation spectrum, taking the form of a flat *spin ice* mode [2]. Correspondingly, we show here that above about 0.25 T, a flat dynamic *kagome ice* mode forms in the excitation spectrum, featuring a "dynamic kagome ice" state [3]. Mean-field calculations using the XYZ Hamiltonian [4,5] adapted for the Nd ion account qualitatively for our observations, although some discrepancies point to the existence of more complex processes. More generally, our study highlights the key role of transverse terms in the physics of pyrochlore magnets. We shall put this point into broader perspective, in the light of recent neutron scattering results obtained in other quantum spin ice candidates as for instance  $Pr_2Zr_2O_7$  [6].

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# Randomness-induced quantum spin liquid behavior in the s=1/2 Heisenberg antiferromagnet on the pyrochlore lattice.

H. Kawamura and K. Uematsu (Osaka Univ.)

In the last decade, experimental quest for the hypothetical "quantum spin liquid" (QSL) state met several candidate materials on certain geometrically frustrated lattices such as triangular and kagome lattices. The former includes organic salts  $\kappa$ -(ET)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub> and EtMe<sub>3</sub>Sb[Pd(dmit)<sub>2</sub>]<sub>2</sub>, while the latter includes herbersmithite CuZn<sub>3</sub>(OH)<sub>6</sub>Cl<sub>2</sub>. These spin-1/2 compounds exhibit no magnetic ordering nor the spin freezing down to very low temperature, while the measured physical quantities mostly exhibit gapless behaviors. We have argued that these compounds might contain significant amount of (effective) quenched randomness or inhomogeneity of varying origin, i.e., the freezing of the charge (dielectric) degrees of freedom in the case of triangular organic salts and the possible Jahn-Teller distortion accompanied by the random substitution of Zn<sup>2+</sup> by Cu<sup>2+</sup> in the case of herbertsmithite, which might be essential in stabilizing the QSL-like behaviors observed experimentally [1-4]. We then proposed as a minimal model the s=1/2 antiferromagnetic Heisenberg model on various geometrically frustrated two-dimensional (2D) lattices, e.g., triangular and kagome lattices with a quenched randomness in the exchange interaction, and demonstrated that, when the randomness exceeds a critical value, the model exhibits a randomness-induced gapless QSL-like state, a "random-singlet state", accompanied by the T-linear low-temperature specific heat widely observed experimentally [1-4]. The random-singlet state, where local spin singlets of varying strengths are formed in a hierarchical manner, might be viewed as an "Anderson-localized" RVB (resonating-valence bond) state. The results seem to provide a consistent explanation of many recent experimental observations.

Next interesting question to be addressed might be that such a randomness-induced QSL state is ever possible also in 3D. In this connection, an experiment observation of the QSL state was recently reported for the s=1/2 pyrochlore magnet Lu<sub>2</sub>Mo<sub>2</sub>O<sub>5</sub>N<sub>2</sub>, containing a significant amount of quenched randomness [5]. Motivated by the experiment, we have studied both zero- and finite-temperature properties of the s=1/2 antiferromagnetic Heisenberg model on the 3D pyrochlore lattice with the random nearest-neighbor exchange coupling. The randomness is introduced via the distribution width  $\Delta$  of the antiferromagnetic nearest-neighbor interaction with the mean J. We then find by means of an exact diagonalization calculation that, while the model exhibits a QSL behavior presumably with a small spin gap in the regular ( $\Delta=0$ ) and weakly random case, on increasing the randomness  $\Delta$  beyond a critical value, it exhibits a "phase transition" into another QSL state with gapless behaviors including the T-linear low-T specific heat, a 3D analogue of the random-singlet state identified for various 2D systems. Thus, the random-singlet state turns out to be possible also in 3D under certain conditions, whose properties are more or less similar to those in 2D. Various other quantities including the susceptibility, the static and the dynamical spin structure factors are computed. On the basis of the obtained data, experimental implications to Lu<sub>2</sub>Mo<sub>2</sub>O<sub>5</sub>N<sub>2</sub> and other related materials are discussed.

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#### 0.8 Kitaev I

Wednesday, 8:30-10:00 Knolle, Halasz, Wu

#### **Dynamics of Kitaev Spin Liquids.**

Johannes Knolle (Imperial College London)

Quantum spin liquids are fascinating because of their unusual properties such as spin fractionalization and long-range entanglement. Unlike conventional symmetry breaking the topological order underlying quantum spin liquids is hard to detect experimentally. At the same time, their fractionalised excitations can be much more characteristic and accessible to regular experiments like inelastic neutron scattering (INS). I will give an overview of the rich physics of the paradigmatic Kitaev Quantum Spin Liquid. Focussing on the dynamic correlations I will discuss which aspects are generic, and which are owed to the exact solubility of the pure Kitaev model.

#### Probing Kitaev spin liquids with resonant inelastic X-ray scattering.

G. Halász (KITP, UC Santa Barbara), N. Perkins (University of Minnesota), B. Perreault (University of Minnesota), J. van den Brink (IFW Dresden)

We propose that resonant inelastic X-ray scattering (RIXS) is an effective probe to detect the fractionalized excitations in two- and three-dimensional Kitaev spin liquids. While the non-spin-conserving RIXS responses are dominated by the gauge-flux excitations and reproduce the inelastic-neutron-scattering response, the spin-conserving (SC) RIXS response picks up the Majorana-fermion excitations and detects whether they are gapless at Dirac / Weyl points, nodal lines, or Fermi surfaces. As a signature of symmetry fractionalization, the SC RIXS response is suppressed around the  $\Gamma$  point for any Kitaev spin liquid on a bipartite lattice.

#### Antiferromagnetic resonance and terahertz continuum in $\alpha$ -RuCl<sub>3</sub>

L. Wu (UC Berkeley & U. Penn), A. Little (UC Berkeley), E. Adape (UC Berkeley), D. Rees(UC Berkeley), P. Lampen-Kelley (ORNL), A. Banerjee (ORNL), D. Mandrus (ORNL), S. Nagler (ORNL), E. Altman (UC Berkeley), J. Orenstein (UC Berkeley)

We report measurements of optical absorption in the zig-zag antiferromagnet  $\alpha$ -RuCl<sub>3</sub> as a function of temperature, T, magnetic field, B, and photon energy,  $\hbar\omega$  in the range  $\sim 0.3$  to 8.3 meV, using time-domain terahertz spectroscopy[1]. Polarized measurements show that 3-fold rotational symmetry is broken in the honeycomb plane from 2 K to 300 K. We find a sharp absorption peak at 2.56 meV upon cooling below the Néel temperature of 7 K at B=0 that we identify as magnetic-dipole excitation of a zero-wavevector magnon, or antiferromagnetic resonance (AFMR). With application of B, the AFMR broadens and shifts to lower frequency as long-range magnetic order is lost in a manner consistent with transitioning to a spin-disordered phase. From direct, internally calibrated measurement of the AFMR spectral weight, we place an upper bound on the contribution to the dc susceptibility from a magnetic excitation continuum. In a most recent study [2], we aim to understand the low field magnon behavior and the spin Hamiltonian, which is the first step to address whether this material hosts exotic fractionalized excitations. I will discuss how many magnons there are below the critical field and the dramatic spectral weight shift between them in various geometries. By combining the linear spin-wave theory, our measurements highly constrain parameters of the spin Hamiltonian.

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O.8. KITAEV I Page 16

#### 0.9 Kitaev II

Wednesday, 10:30-12:00 Banerjee, Valenti, Kee

#### Magnetic disorder, order and models of Kitaev candidate alpha-RuCl<sub>3</sub>.

P. Kelley (UTK), C. Balz (ORNL), M. Stone (ORNL), B. Winn (ORNL), Y. Liu (ORNL), J. Yan (ORNL), C. Bridges (ORNL), D. Mandrus (UTK), J. Knolle (Imperial), R. Moessner (MPI-Dresden), S. Nagler (ORNL)

The layered honeycomb magnet alpha-RuCl3 has emerged as a candidate material for realizing Kitaev physics. The effective spin Hamiltonian contains Kitaev, Heisenberg, and off-diagonal terms leading to an ordered ground state in zero field. At the same time, inelastic neutron scattering measurements show that, in addition to spin waves associated with the ordered state, the excitation spectrum contains a scattering continuum expected for fractionalized excitations such as those extant in the Kitaev quantum spin liquid. An applied field in the honeycomb plane suppresses the magnetic order. In this talk, I will describe the comprehensive measurements of the directional dependence of the zero-field static susceptibility, as well as field-dependent dynamic susceptibility, which show a complex behavior spin behaviour and reveal a new field-dependent phase. I will also closely examine the low-energy neutron spectrum both with and without field to distinguish the effects of order, disorder, and non-linearity. The results, taken together, helps us identify critical ways to constrain the spin Hamiltonian.

REFERENCES

#### Field-induced phases in generalized Kitaev models and materials

Roser Valentí (ITP, Goethe University Frankfurt)

By using a combination of density functional theory, exact diagonalization and semi-classical calculations we present a detailed analysis of possible field-induced phases obtained by adding to the Kitaev model further interaction terms. In particular we discuss the possibility of the appearance of topologically non-trivial field-induced spin liquid phases and the implications of these results in relation to the most studied  $\alpha$ -RuCl<sub>3</sub>[1,2].

Work done in collaboration with Steve Winter, Kira Riedl, David Kaib and Radu Coldea.

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- [2] D. Kaib et al. (in preparation).

#### Path to stable quantum spin liquids in spin-orbit coupled correlated materials

H. Y. Kee (Univ. of Toronto), A. Catuneanu (Univ. of Toronto), Y. Yamaji (Univ. of Tokyo), G. Wachtel (Univ. of Toronto), Y. B. Kim (Univ. of Toronto)

The spin liquid phase is one of the prominent strongly interacting topological phases of matter whose unambiguous confirmation is yet to be reached despite intensive experimental efforts on numerous candidate materials. One challenge is to formulate realistic theoretical models for these materials and interpreting the corresponding experimental data. We study a generic spin model for the spin-orbit coupled honeycomb materials[1], and show numerical evidence for the existence of an extended quantum spin liquid region, which is possibly connected to the Kitaev spin liquid state[2]. Experimental implications to honeycomb iridates and RuCl3 are discussed.

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0.9. KITAEV II Page 17

#### 0.10 Kitaev III

Wednesday, 1:30-3:00 Rousochatzakis, Kim, Ruiz

#### Quantum spin liquid in the semiclassical regime

I. Rousochatzakis (UMN), Y. Sizyuk (UMN) and N. Perkins (UMN)

According to received wisdom, quantum spin liquids can arise in frustrated magnets with low spin S, where strong quantum fluctuations act to destabilize conventional, magnetically ordered states. Here we present a magnet that has a  $Z_2$  quantum spin liquid ground state already in the semiclassical, large-S limit. The state has both topological and symmetry related ground state degeneracy, and two types of gaps, a 'magnetic flux' gap that scales linearly with S and an 'electric charge' gap that drops exponentially in S. The magnet is described by the spin-S version of the spin-S kitaev honeycomb model, which has been the subject of intense studies in correlated electron systems with strong spin-orbit coupling, and in optical lattice realizations with ultracold atoms. The results apply to both integer and half-integer spins. I. Rousochatzakis, Y. Sizyuk and N. Perkins, arXiv:1706.03756

#### Theory of a quantum spin liquid in hydrogen-intercalated honeycomb iridate, H<sub>3</sub>LiIr<sub>2</sub>O<sub>6</sub>

Yong-Baek Kim (University of Toronto)

We propose a theoretical model for a gapless spin liquid phase that may have been observed in a recent experiment on  $H_3 \text{LiIr}_2 O_6$ . Despite the insulating and non-magnetic nature of the material, the specific heat coefficient  $C/T \sim 1/\sqrt{T}$  in zero magnetic field and  $C/T \sim T/B^{3/2}$  with finite magnetic field B have been observed. In addition, the NMR relaxation rate shows  $1/(T_1T) \sim (C/T)^2$ . Motivated by the fact that the interlayer/in-plane lattice parameters are reduced/elongated by the hydrogen-intercalation of the parent compound  $\text{Li}_2\text{IrO}_3$ , we consider four layers of the Kitaev honeycomb lattice model with additional interlayer exchange interactions. It is shown that the resulting spin liquid excitations reside mostly in the top and bottom layers of such a layered structure and possess a quartic dispersion. In an applied magnetic field, each quartic mode is split into four Majorana cones with the velocity  $v \sim B^{3/4}$ . We suggest that the spin liquid phase in these "defect" layers, placed between different stacking patterns of the honeycomb layers, can explain the major phenomenology of the experiment, which can be taken as evidence that the Kitaev interaction plays the primary role in the formation of a quantum spin liquid in this material.

REFERENCE: Kevin Slagle, Wonjune Choi, Li Ern Chern, Yong Baek Kim, arXiv:1710.01307

#### Hidden ferromagnetism in the Kitaev honeycomb iridates.

A. Ruiz (UC Berkeley), G. Lopez (UC Berkeley), M. Vranas (UC Berkeley) and J. G. Analytis (UC Berkeley) ABSTRACT TEXT.

A unique feature of 5d materials is the fact that spin-orbit  $\lambda_{SOC}$  and Coulomb interactions U are of comparable strength. In the honeycomb iridates, this leads to strongly anisotropic, Ising-like exchange between neighboring spin-1/2 moments. Such interactions couple each spin to orthogonal components of the three neighboring spins and, as a consequence, no single exchange direction can be simultaneously satisfied, leading to strong frustration closely approximated by the Kitaev Hamiltonian. So far, all potential Kitaev materials have been found to order at low temperatures, eluding the sought-after QSL state. However, most experiments suggest that Kitaev exchange is the dominant spin interaction in these systems with small contributions from a direct Heisenberg and a symmetric off-diagonal exchange term. The intricate balance of these different energy scales dictates the nature of the observed ground state while external perturbations such as an applied magnetic field, can tilt the balance into a nearby state. In this work, we present thermodynamic evidence for a thus far overlooked ferromagnetic transition in all members of the Kitaev honeycomb iridate family which provides an opportunity to understand the true microscopic Hamiltonian and to construct the correct phase diagram that describes these compounds.

0.10. KITAEV III Page 18

#### 0.11 Kitaev IV

Wednesday, 4:30-6:00 Pollmann, Udagawa, Shimizu

#### Efficient simulation of the dynamics in frustrated spin systems.

Frank Pollmann (TUM, Munich), Ruben Verresen (TUM, Munich), Matthias Gohlke (MPIPKS, Dresden), Roderich Moessner (MPIPKS, Dresden)

Dynamical response functions encode characteristic features of the emergent excitations in frustrated magnets. We introduce a matrix-product state based method to efficiently obtain these dynamical response functions for general two-dimensional lattice Hamiltonians. First, we apply this method to different phases of the Kitaev-Heisenberg model. Here we find significant broad high energy features beyond spin-wave theory even in the ordered phases proximate to spin liquids. This includes the phase with zig-zag order of the type observed in  $\alpha$ -RuCl3, where we find high energy features like those seen in inelastic neutron scattering experiments [1]. Second, we study the stability of magnon excitations in Heisenberg antiferromagnets.

[1] M. Gohlke, R. Verresen, R. Moessner, and and F. Pollmann, Phys. Rev. Lett. 119, 157203 (2017).

#### Vison resonance in Kitaev spin liquids

Masafumi Udagawa (Gakushuin Univ.)

Recently, Kitaev's model is drawing considerable attention as a platform to study quantum spin liquid, and several compounds have been proposed as promising stages to realize this unusual spin liquid state. Among many non-trivial properties, it is remarkable that the spin liquid phases host unusual excitations: spins are fractionalized into itinerant Majoranas and visions, and the latter behave as abelian/non-abelian anyons. The understanding of these elementary excitations should be essential to identifying Kitaev spin liquid phases in actual materials. Indeed, in RuCl<sub>3</sub>, continuum spectra have been observed in inelastic neutron scattering [1] and Raman spectroscopy [2], implying the contribution of itinerant Majoranas. Meanwhile, there have been no evidence so far, regarding the presence of visons, and especially their nontrivial statistics.

In this contribution, we examine possible experimental signatures of visons. For this purpose, we present an exact analytical formula of the real-time spin correlation in this system, and discuss the dynamical properties of this system. In particular, we will consider the effect of impurity, and address the zero-energy resonance and its observation through spin-lattice relaxation rate [3], which can be attributed to the "vison zero mode" in the vicinity of diluted site. Furthermore, we incorporate the effect of perturbation off the Kitaev's integrable limit into the analytical solution, and address the dynamics of visons, and discuss how their dynamics is reflected in experimental observables, such as dynamical spin structure factor.

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- [3] M. Udagawa, in preparation.

#### Quantum Criticality of Kitaev Spin Liquid.

Y. Shimizu (Nagoya Univ.), Y. Nagai (Nagoya Univ.), M. Itoh (Nagoya Univ.), J. Yoshitake (Tokyo Univ.), J. Nasu, (Tokyo Tech. Univ.) and Y. Motome (Tokyo Univ.)

The ruthenium trichloride serves as a promising candidate of the Kitaev quantum spin liquid induced by magnetic field. Here we present a comprehensive nuclear magnetic resonance study on a high quality single crystal across the quantum phase transition. The dynamical critical exponents are distinct from the conventional two dimensional Ising model at zero field, reflecting the emergent dynamics of itinerant Majorana fermions. As topological flux evolves at high fields, the gap opens for the dynamical spin correlations, in excellent agreement with the Kitaev's prediction of the anyons.

0.11. KITAEV IV Page 19

#### 0.12 Kitaev V

Thursday, 8:30-10:00 Matsuda, Motome, Lee

#### Majorana signatures in Kitaev quantum spin liquids

Yukitoshi Motome (Univ. of Tokyo)

In this talk I will give an overview on our theoretical studies on finite-temperature properties in the Kitaev model. The Kitaev model is a spin S = 1/2 model with bond-dependent Ising-type interactions, originally introduced on a honeycomb lattice and later extended to other tricoordinate lattices. The importance of this model is twofold: one is that it is exactly soluble and provides quantum spin liquids in the ground state [1], and the other is that it is potentially realized in some spin-orbit entangled Mott insulators [2]. Although the model has stimulated both theoretical and experimental understanding of quantum spin liquids in the past decade, it remains elusive how to identify the signatures of the Kitaev quantum spin liquids in the candidate materials. The key aspect is the fractionalization; in the Kitaev model elementary spin excitations are fractionalized into Majorana fermions. In order to clarify how such fractional excitations manifest themselves in experimentally observable quantities, we have investigated the static and dynamical properties of the Kitaev model at finite temperature, by developing new numerical techniques based on a Majorana fermion representation. We have unveiled the fingerprints of Majorana fermions in temperature and energy dependences of various physical observables, such as the specific heat [3,4], magnetic susceptibility, NMR relaxation rate, dynamical spin structure factor [5-8], Raman scattering [9], and thermal transport [10,11]. We will discuss the results in comparison with recent experimental data for the candidate materials. This work is supported by Grant-in-Aid for Scientific Research under Grants No. JP15K13533 and No. JP16H02206. Parts of the numerical calculations were performed in the supercomputing systems in ISSP, the University of Tokyo.

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#### Thermal Hall effect in a Kitaev spin liquid: A possible signature of Majorana chiral edge current

Yuji Matsuda (Department of Physics, Kyoto University, Japan)

The Kitaev quantum spin liquid displays the fractionalization of quantum spins into Majorana fermions. The emergent Majorana edge current is predicted to manifest itself in the form of a finite thermal Hall effect, a feature commonly discussed in topological superconductors. Here we report on thermal Hall conductivity  $\kappa_{xy}$  measurements in  $\alpha$ -RuCl<sub>3</sub>, a candidate Kitaev magnet with the two-dimensional honeycomb lattice. In a spin-liquid (Kitaev paramagnetic) state below the temperature characterized by the Kitaev interaction  $J_K/k_B \sim 80$  K, positive  $\kappa_{xy}$  develops gradually upon cooling, demonstrating the presence of highly unusual itinerant excitations [1]. Although the zero-temperature property is masked by the magnetic ordering at  $T_N=7$  K, the sign, magnitude, and T-dependence of  $\kappa_{xy}/T$  at intermediate temperatures follows the predicted trend of the itinerant Majorana excitations. We also report the thermal Hall effect in the tilted magnetic field, where the magnetic ordering is completely suppressed[2].

In collaboration with Y. Kasahara, T. Ohnishi (Kyoto University), K. Sugii, M. Shimozawa, M. Yamashita, T. Shibauchi, Y. Motome (University of Tokyo), N. Kurita and H. Tanaka (Tokyo Institute of Technology)

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#### In-plane thermal conductivity and magnetic torque study in 2D honeycomb lattice magnets

Minhyea Lee(Presenter, U. Colorado Boulder), Chris A. Pocs, Ian A. Leahy (U.Colorado Boulder), Bruce Normand (PSI, Switzerland) S.-W. Doh, K.-Y. Choi (Chung-Ang Univ., South Korea), E. S. Choi and D. Graf (NHMFL)

Thermal transport measurement is one of key experimental probes to study insulating quantum magnets and their phase diagram. In principle, thermal conductivity is proportional to the product of thermal diffusion constant and specific heat but is contributed only by mobile excitations not by localized ones. In this talk, I will present the thermal conductivity and the torque magnetization results on quasi 2D honey comb lattice magnets - RuCl<sub>3</sub>, CrCl<sub>3</sub> and Na<sub>2</sub>IrO<sub>3</sub>. Different contributions to thermal conductivity to the complex temperature and magnetic field dependence will be discussed in the relation to the torque magnetization.

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# 0.13 Frustrated Magnetism I

Thursday, 10:30-12:30 Rougemaille, Becca, Honecker, Poilblanc

# Artificial spin systems as experimental simulators of frustrated magnets: from the fragmentation of magnetization to the six vertex model

N. Rougemaille (Institut NEEL, Grenoble, France), Y. Perrin (Institut NEEL, Grenoble, France), I.-A. Chioar (Institut NEEL, Grenoble, France), V.-D. Nguyen (Institut NEEL, Grenoble, France), M. Hehn (Institut Jean Lamour, Nancy, France), D. Lacour (Institut Jean Lamour, Nancy, France), F. Montaigne (Institut Jean Lamour, Nancy, France), A. Locatelli, (ELETTRA synchrotron, Trieste, Italy) T. O. Mentes (ELETTRA synchrotron, Trieste, Italy), B. Santos Burgos (ELETTRA synchrotron, Trieste, Italy) and B. Canals (Institut NEEL, Grenoble, France)

Complex architectures of nanostructures are routinely elaborated using bottom-up or nanofabrication processes. This technological capability allows scientists to engineer materials with properties that do not exist in nature, but also to manufacture model systems permitting the exploration of fundamental issues in condensed matter physics. One- and two-dimensional frustrated arrays of magnetic nanostructures are one class of systems for which theoretical predictions can be tested and revisited experimentally. These systems have been the subject of intense research in the last few years and allowed the investigation of a rich physics, including the study of the extensively degenerate ground-state manifolds of spin ice systems, the evidence of new magnetic phases in purely two-dimensional lattices, and the observation of pseudo-excitations involving classical analogues of magnetic monopoles. This talk aims at providing two examples of artificial spin systems in which the low-energy physics of two exotic Ising models was probed. The first one is related to the seminal six vertex model. More specifically, we show that a scan through the phase diagram of the six vertex model can be achieved experimentally, provided that the artificial spin system is designed appropriately [1]. In particular, the symmetric point of the square ice is recovered, and signatures of an algebraic Coulomb spin liquid are observed. Because of the experimental procedure used to reach this low-energy physics, quasi-particles are trapped in a disordered manifold, pointing to the need of thermal systems, but also emphasizing that these systems may be well suited for studying out-of-equilibrium relaxation of monopole-monopole pairs. The second example refers to a recent proposal, the fragmentation of magnetization [2], in an Ising kagome model. Here, we report the observation of this intriguing phenomenon, which corresponds to the splitting of the local degree of freedom into two channels, one ordering at low effective temperatures, in an antiferromagnetic all-in all-out fashion despite the ferromagnetic nature of the system, and the other, building a Coulomb-like low-energy manifold, inside which the magnetic equivalent of the Kirchhoff law at each node of the kagome lattice is fulfilled [3].

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#### Dynamical structure factor of frustrated spin models: a variational Monte Carlo approach

Federico Becca (CNR and SISSA)

The spin dynamical structure factor is computed within a variational framework to study frustrated Heisenberg models in one and two dimensions. Starting from Gutzwiller-projected fermionic wave functions, the low-energy spectrum is constructed by considering two-spinon excitations. A benchmark of this approach on the one-dimensional  $J_1-J_2$  model is considered. Here, an excellent description of both the gapless and gapped (dimerized) phases is obtained, also describing the incommensurate structure for large frustrating ratios  $J_2/J_1>0.5$  [1]. In the square lattice, we are able to unveil the dynamical signatures of the transition between the Neel and the (gapless) spin-liquid phases that takes place for  $J_2/J_1\approx 0.45$ . In particular, by increasing the frustration, the magnon excitation at  ${\bf q}=(\pi,0)$  and  $(0,\pi)$  broadens, suggesting the tendency towards a spin fractionalization. In addition, its energy softens, indicating the presence of

gapless states at the transition and within the spin-liquid phase. [2] Future applications will focus on the Heisenberg model on the Kagome lattice, as well as further benchmarks on the Kitaev model, where the exact calculation of the dynamical structure factor is possible [3].

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[2] F. Ferrari and F. Becca, in preparation.
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#### Quantum-Monte-Carlo Approach to the Thermodynamics of Highly Frustrated Spin-1/2 Antiferromagnets.

Andreas Honecker
(Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France),
Ido Niesen, Philippe Corboz
(Institute for Theoretical Physics, University of Amsterdam, The Netherlands),
Bruce Normand
(Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Switzerland),
Frédéric Mila
(Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland),
Jonas Stapmanns, and Stefan Wessel
(Institut für Theoretische Festkörperphysik, RWTH Aachen University, Germany)

Highly-frustrated antiferromagnets are notorious for giving rise to a severe sign problem in conventional Quantum-Monte-Carlo (QMC) simulations. However, recently progress has been made for the thermodynamics of certain models that allow rewriting in an appropriate "cluster" basis, notably a dimer basis [1,2]. Here we go beyond these previous studies and assess the range of applicability of such an approach to certain two-dimensional highly frustrated quantum antiferromagnets.

Firstly, we investigate the two-dimensional spin-1/2 Shastry-Sutherland model for  $SrCu_2(BO_3)_2$ . This model is well-known for an exact dimer ground state owing to an orthogonal arrangement of its constituting dimers. We assess the range of applicability of the QMC approach in the dimer basis for the two-dimensional spin-1/2 Shastry-Sutherland model by comparing it to complementary exact diagonalization and high-temperature series, with a particular focus on the specific heat C and the magnetic susceptibility  $\chi$  in the parameter regime relevant to  $SrCu_2(BO_3)_2$ . We also consider a generalization of the Shastry-Sutherland model that in another limit is topologically equivalent to the fully frustrated square lattice bilayer. For the fully frustrated square lattice bilayer, QMC simulations in the inter-layer spin dimer basis become actually sign free. This enables us to investigate the finite-temperature phase diagram of the fully frustrated square lattice bilayer in detail, in particular we can follow a T=0 discontinuous quantum phase transition between an inter-layer singlet phase and an antiferromagnetic phase to finite temperature.

- [1] A. Honecker, S. Wessel, R. Kerkdyk, T. Pruschke, F. Mila, and B. Normand, *Thermodynamic Properties of Highly Frustrated Quantum Spin Ladders: Influence of Many-Particle Bound States*, Phys. Rev. B **93**, 054408 (2016).
- [2] S. Wessel, B. Normand, F. Mila, and A. Honecker, *Efficient Quantum Monte Carlo Simulations of Highly Frustrated Magnets: The Frustrated Spin-1/2 Ladder*, SciPost Phys. **3**, 005 (2017).

#### Search for topological SU(2) chiral spin liquids using iPEPS

Didier Poilblanc (CNRS & Université de Toulouse, France)

It was shown that a chiral generalization of the spin-1/2 resonating valence bond (RVB) state can be written as a simple D=3 projected entangled pair state (PEPS) [1,2], suggesting that the PEPS framework is an ideal scheme to search for chiral spin liquids in simple quantum spin Hamiltonians. A simple spin-1/2 frustrated antiferromagnetic Heisenberg model (AFHM) on the square lattice - including chiral plaquette cyclic terms - was argued to host a bosonic Kalmeyer-Laughlin (KL) fractional quantum Hall ground state. Here, we construct generic families of chiral PEPS with

low bond dimension which, upon optimization, provide better variational energies (obtained by infinite-PEPS techniques) than the KL ansatz [3]. The optimal PEPS exhibits chiral edge modes described by the Wess-Zumino-Witten SU(2)<sub>1</sub> model, as expected for the KL spin liquid. However, we find evidence that, in contrast to the KL state, the PEPS spin liquids have power-law dimer-dimer correlations and exhibit a gossamer long-range tail in the spin-spin correlations. Extensions to spin-1 chiral AFHM [4] will also be discussed. Various implications of these results will be outlined.

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  - [2] Chiral topological spin liquids with projected entangled pair states, Didier Poilblanc, J. Ignacio Cirac, Norbert Schuch, Phys. Rev. B 91, 224431 (2015);
- [3] Investigation of the chiral antiferromagnetic Heisenberg model using iPEPS, Didier Poilblanc, Phys. Rev. B 96, 121118 (R) (2017);
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# 0.14 Kagome I

Friday, 8:30-10:00 Xiang, Kao, Fennell

#### Gapless Spin-Liquid Ground State in the S=1/2 Kagome Antiferromagnet

T. Xiang<sup>1</sup>, H. J. Liao<sup>1</sup>, Z. Y. Xie<sup>2</sup>, B. Normand<sup>3</sup>

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<sup>3</sup>Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

The defining problem in frustrated quantum magnetism, the ground state of the nearest-neighbor spin 1/2 antiferromagnetic Heisenberg model on the kagome lattice, has defied all theoretical and numerical methods employed to date. We apply the formalism of tensor-network states, specifically the method of projected entangled simplex states, which combines infinite system size with a correct accounting for multipartite entanglement. By studying the ground-state energy, the finite magnetic order appearing at finite tensor bond dimensions, and the effects of a next-nearest-neighbor coupling, we demonstrate that the ground state is a gapless spin liquid.

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#### A two-dimensional classical spin liquid in quantum kagome ice.

Y.-J. Kao (National Taiwan University) and K.-H. Wu (National Taiwan University)

We re-examine the spin-1/2 XYZh model on a kagome lattice using quantum Monte-Carlo (QMC) simulations. Recent studies show that there exists a quantum kagome ice state with no magnetic orders that is proposed to be a  $\mathbb{Z}_2$  quantum spin liquid (QSL) [1]. Our topological entanglement entropy results indicate, however, that this state does not have a topological order. The low temperature thermal entropy also matches the residual entropy of a classical kagome ice. Simulations from an effective classical model reproduce the static correlation functions observed in the QMC simulation. We argue that to the lowest temperature reached, the state remains disordered with classical kagome ice signatures, and is not a  $\mathbb{Z}_2$  quantum spin liquid. The connection with the disorder-by-disorder phenomena in the transverse Ising antiferromagnetic model on a kagome lattice will be discussed.

[1] J. Carrasquilla, Z. Hao, and R. G. Melko, Nat. Comm. 6, 7421 (2014); Y.-P. Huang and M. Hermele, Phys. Rev. B 95, 075130 (2017).

#### Multiple Coulomb phase in the fluoride pyrochlore CsNiCrF<sub>6</sub>.

T. Fennell (PSI), M. J. Harris (Edinburgh), S. Calder (ORNL), M. Ruminy (PSI), M. Boehm (ILL), P. Steffens (ILL), M.-H. Lemée-Cailleau (ILL), O. Zaharko (PSI), A. Cervellino (PSI), S. T. Bramwell (UCL)

Coulomb phases can be constructed for local degrees of freedom obeying an ice rule on the pyrochlore lattice [1]. Using diffuse and single crystal neutron and powder x-ray scattering, we identify a structural Coulomb phase, or charge ice [2], formed by the Ni<sup>2+</sup> and Cr<sup>3+</sup> cations in CsNiCrF<sub>6</sub>. The diffuse scattering indicates that not only do the cations form a configurational structural ice, but they dictate local distortions of the (Ni/Cr)F<sub>6</sub> octahedra, which also inherit the Coulomb phase correlations. The resulting exchange disorder can be mapped to a fully-packed loop model [3,4]. Despite this disorder, diffuse and inelastic magnetic neutron scattering show that the spins also form a Coulomb phase, whose correlations and dynamics have much in common with those of the canonical pyrochlore Heisenberg antiferromagnet [5].

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# 0.15 Kagome II

Friday, 10:30-12:00 Lake, Reuther, Ralko

#### Exploration of the quantum spin liquid state in Ca<sub>10</sub>Cr<sub>7</sub>O<sub>28</sub>.

B. Lake (Helmholtz Zentrum Berlin; Technical University Berlin, Germany), C. Balz (Helmholtz Zentrum Berlin, Germany; Oak Ridge National Lab, USA), A.T.M.N. Islam (Helmholtz Zentrum Berlin, Germany), U. Tutsch (Goethe University, Frankfurt, Germany), Y. Matsuda (Kyoto University, Japan), L. Opherden (Helmholtz Zentrum Dresden Rossendorf, Germany; Technical University Dresden, Germany), T. Herrmannsdörfer (Helmholtz Zentrum Dresden Rossendorf, Germany), J.A. Rodriguez-Rivera (NIST Center for Neutron Research; University of Maryland, USA).

 $Ca_{10}Cr_7O_{28}$  is a new quantum spin liquid where the magnetic  $Cr^{5+}$  ions  $(S-\frac{1}{2})$  form breathing Kagome bilayers. Both kagome layers consist of alternating ferromagnetic and antiferromagnetic corner-sharing triangles and the two layers are stacked so that the ferromagnetic triangles lie on top of antiferromagnetic triangles and vice versa. Previous measurements revealed the absence of long-range magnetic order and the presence of persistent spin dynamics in the ground state. Here we present a detailed exploration of the ground state and excitations using magnetisation, heat capacity, thermal conductivity and inelastic neutron scattering. The heat capacity and thermal conductivity are linear in temperature suggesting the presence of a gapless spinon Fermi surface. The excitations are diffuse revealing the presence of spinon continuua, and they form a distinct pattern that evolves gradually with energy. The data is compared to theoretical models for the spinon Fermi surface. Together these results provide strong evidence that  $Ca_{10}Cr_7O_{28}$  is a gapless Z2 quantum spin liquid.

#### A theory perspective on the spin liquid candidate material PbCuTe $_2$ O $_6$ .

J. Reuther (Helmholtz-Zentrum Berlin and Freie Universität Berlin), S. Chillal (Helmholtz-Zentrum Berlin), Y. Iqbal (Indian Institute of Technology Madras), H. Jeschke (Okayama University), R. Thomale (University of Würzburg) and B. Lake (Helmholtz-Zentrum Berlin)

The compound PbCuTe<sub>2</sub>O<sub>6</sub>, featuring a 3D hyperkagome network of spin-1/2 Cu<sup>2+</sup> ions, represents a promising new candidate to realize a quantum spin liquid. Experimentally, PbCuTe<sub>2</sub>O<sub>6</sub> shows no signature of static magnetic order accompanied by diffuse (spinon-like) spheres in the measured spin-structure factor. To determine the system's spin Hamiltonian and to understand the microscopic origin of the non-magnetic ground state we employ a combination of ab initio DFT and pseudofermion functional renormalization group (PFFRG) calculations. Our DFT results indicate that the system exhibits two dominant antiferromagnetic Heisenberg spin interactions  $J_1$  and  $J_2$  on crystallographically inequivalent bonds which are of almost the same strength. While  $J_1$  couples the spins into isolated triangles, the  $J_2$  interactions form a hyperkagome lattice. The combination of both couplings creates a highly frustrated network of corner-sharing triangles which we dub a hyper-hyperkagome lattice'. Longer-range interactions  $J_3$  and  $J_4$  are found to be considerably smaller than  $J_1$  and  $J_2$ . Simulating this model with PFFRG we confirm the non-magnetic nature of its ground state and reproduce the measured spin structure factor with remarkable accuracy. The absence of long-range magnetic order can be understood from the classical  $J_1$ - $J_2$  only model, which features an infinite set of degenerate ground states through which the system can fluctuate. We propose that such fluctuations destabilize any static magnetic order even in the quantum spin-1/2 case.

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#### Importance of virtual singlets in RVB theory of quantum spin liquids.

A. Ralko (Néel, France), F. Mila (EPFL, Switzerland) and I. Rousochatzakis (SPA, USA)

It is well known that the low-energy sector of quantum spin liquids and other magnetically disordered systems is governed by short-ranged resonating-valence bonds. Here, we will show that the standard minimal truncation to the nearest neighbor valence-bond basis fails completely even for systems where it should work the most, according to received wisdom. This paradigm shift is demonstrated for both the quantum spin-1/2 square-kagome [1] and kagome [2] lattices, where the strong geometric frustration prevents magnetic ordering down to zero temperature. In the former, the shortest tunneling events bear the strongest longer-range fluctuations, leading to amplitudes that do not drop exponentially with the length of the loop, and to an unexpected loop-six valence-bond crystal, which is otherwise very high in energy at the minimal truncation level. In the latter, we will show from preliminary results [3] how the virtual singlets help in understanding the complex structure of the spin liquid of the RVB description of spin-1/2 kagome antiferromagnets by evidencing the proximity of a diamond-like crystal and making comparison with other numerical methods such as DMRG.

[1] A. Ralko and I. Rousochatzakis, Phys. Rev. Lett. 115 167202 (2015)
[2] I. Rousochatzakis, Y. Wan, O. Tchernyshyov and F. Mila, PRB 90 100406(R) (2014)
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# 0.16 Frustrated Magnetism II

Friday, 1:30-3:00 Broholm, Mendels, MacDougall

#### Frustrated Magnetism in Pyrochlore Fluorides\*.

Collin Broholm (Johns Hopkins)

Recently introduced by Krizan and Cava, a family of pyrochlore fluorides of the form NaCaM2F7 and NaSrM2F7 (M=Fe, Mn, Ni, Co) offers exciting opportunities to explore frustrated quantum magnetism [1-3]. The Curie-Weiss temperatures are in the 100 K range, large single crystals can be synthesized by a modified Bridgman method, and both quantum and classical, isotropic and anisotropic magnetism is possible depending on the transition metal ion. I shall review the bulk magneto-thermal properties of the series and then describe neutron scattering experiments probing spin correlations in NaCaNi2F7 [4] and NaSrMn2O7 [5]. Rather than magnetic ordering both compounds exhibit a low temperature spin-glass-like phase. They have an isotropic spin Hamiltonians but different spin quantum numbers and different exchange disorder, which allows for an informative comparative study.

\*Supported by U.S. DoE Basic Energy Sciences, DE-FG02-08ER46544 and by the Gordon and Betty Moore foundation GBMF 4532; [1] "NaCaCo2F7: A single-crystal high-temperature pyrochlore antiferromagnet," J. W. Krizan and R. J. Cava, Phys. Rev. B 89, 214401 (2014); [2] "NaCaNi2F7: A frustrated high-temperature pyrochlore antiferromagnet with S=1 Ni2+," J.W. Krizan and R.J. Cava, Phys. Rev. B 92, 014406 (2015); [3] "NaSrMn2F7, NaCaFe2F7, and NaSrFe2F7: Novel single crystal pyrochlore antiferromagnets," M.B. Sanders, J.W. Krizan, K.W. Plumb, T.M. McQueen, and R.J. Cava, J. Phys.: Condens. Matter 29, 045801 (2017); [4] "Continuum of quantum fluctuations in a three-dimensional S=1 Heisenberg magnet," K. W. Plumb, Hitesh J. Changlani, A. Scheie, Shu Zhang, J. W. Kriza, J. A. Rodriguez-Rivera, Yiming Qiu, B. Winn, R. J. Cava, and C. L. Broholm, arXiv:1711.07509; [5] A. Scheie et al. unpublished (2018).

#### Low- $T^{\ 17}{ m O}$ NMR study of herbertsmithite crystals.

P. Mendels (Univ. Paris-Sud), P. Khuntia (I.I.T. Madras), Q. Barthélémy (Univ. Paris-Sud), F. Bert (Univ. Paris-Sud), A. Legros (Univ. Paris-Sud), M. Velazquez (ICMCB, CNRS Bordeaux).

Herbertsmithite  $\operatorname{ZnCu_3}(OH)_6\operatorname{Cl_2}$  has been known for long as the best representative of spin liquid physics for the Heisenberg model on a quantum kagome lattice. While quasi-free Cu on Zn sites mask the signature of the kagome physics at low-T in most experimental techniques, typically T < J/10, one can take advantage of the strong coupling of O to the kagome Cu's to track this physics through  $^{17}O$  NMR, see e.g. refs.[1,2,3]. Working on high quality single crystals considerably improved the accuracy of NMR measurements and its ability to address fundamental issues such as the existence of a gap or not and the class of models relevant to describe the ground state of herbertsmithite. However the greatest challenge in such experiments to reach firm conclusions about the low T kagome physics is still to discriminate between what belongs to kagome Cu's and what is the counterpart induced by defects. We have mapped out in detail the latter contribution and could then isolate the  $^{17}O$  NMR spectral signature of kagome Cu's. Neither in our shift

measurements nor in our relaxation studies we find any hint of a gap. On the contrary, we conclude that the susceptibility is finite and independent of the field in the range 3.1 - 12 Teslas. The relaxation varies linearly with temperature down to 1.2 K. We could reproduce the results obtained on powder samples in [3] and confirm the opening of a gap at sub-kelvin temperatures -e.g 0.7 K under 6.6 T.

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#### Pauling entropy and deviation from the dipole-ice model in a spinel spin-ice candidate

G. MacDougall (UIUC), D. Reig-i-Plessis (UIUC), A. Aczel (ORNL), S. van Geldern (UIUC), D. Kochkov (UIUC) and B. Clarke (UIUC)

The pyrochlore structure has long been the rock bed of research into spin ice materials, magnetic monopoles and, more recently, the search for three-dimensional quantum spin liquid states. This has included studies into dozens of different materials, but largely restricted to the 227 rare-earth oxides. Here, I will report on a new family of rare-earth spinel materials,  $\operatorname{Mg} R_2 \operatorname{Se}_4 R \in \{Ho^{3+}, Er^{3+}, Tm^{3+}, Yb^{3+}\}$ , where magnetic moments comprise an undistorted cubic pyrochlore structure, with a local crystal field environment which is distinct from the 227 analogues. I will present inelastic neutron scattering results which allow us to exactly determine the local crystal field spectrum and comment on the wavefunctions and spin anisotropy associated with the low-energy multiplets. I will further show magnetization, heat capacity and neutron powder diffraction data, which reveal a wide variety of behaviors, ranging from order to glassiness to spin ice states. Of particular interest is the material  $\operatorname{MgEr}_2\operatorname{Se}_4$ , which has perfect Ising anisotropy in the ground state

Kramers doublet, spin correlations, and residual Pauling entropy all indicative of a classical spin ice state at low temperature. Intriguingly however, the measured heat capacity deviates significantly from expectations for the traditional dipole-ice model, which may be associated with transverse coupling terms seeded by the observed dipole-octupole form of the Kramers doublet. We will present this data, and discuss them in the context of the current literature and the possibility of quantum spin liquid behavior in this material at lower temperatures. This work was supported by the National Science Foundation under grant no DMR-1455264-CAR.

# 0.17 Intinerant Magnets

Friday, 4:30-6:00 Savary, Sibille, Lee

#### Singular Angular Magnetoresistance and Spontaneous Symmetry Breaking in a Magnetic Nodal Semimetal.

L. Savary (ENS Lyon, CNRS), T. Suzuki (MIT), J.-P. Liu (KITP), J.W. Lynn (NIST), L. Balents (KITP) and J.G. Checkelsky (MIT)

Transport coefficients are incisive experimental probes of the low energy, long wavelength properties of correlated electron systems often useful for mapping hidden phases with distinct symmetries. Here we report a new transport signature of spontaneous symmetry breaking in a magnetic Weyl semimetal in the form of singular angular magnetoresistance (SAMR). This angular response approaching 1000% radian<sup>-1</sup> is confined along the high symmetry axes with a full width at half maximum of less than 1°, significantly sharper than previously observed in bulk magnets. The SAMR phenomenon is explained theoretically as an effect due to controllable high resistance domain walls, arising as a consequence of magnetic point group symmetry breaking strongly coupled to a nearly nodal electronic structure. A theoretical model, based on crystallography and magnetic anisotropy, agrees well with the phase diagram mapped experimentally by SAMR, and predicts a spin structure and magnetic phase boundaries consistent with corresponding neutron scattering and thermodynamic measurements, respectively. This study offers a blueprint for engineering magnetic materials with unprecedented angular sensitivity by lattice and site symmetries.

#### Investigations on quantum effects in some rare-earth pyrochlore oxides.

Romain Sibille (Paul Scherrer Institut)

Rare-earth pyrochlore oxides have been a remarkable source of complex magnetic phases for more than two decades [1]. Some of these phases feature short-range correlated states analogous to a Coulomb phase and give rise to emergent quasiparticle excitations. Although cases like the classical spin ice are reasonably well understood, the theoretical expectation is that quantum fluctuations lead to novel phases that are quantum spin liquids (QSLs) [2]. In such cases, the magnetic moments evade classical long-range order to form an exotic state that is quantum entangled and coherent over macroscopic length scales. In particular, the quantum spin ice (QSI) is an appealing proposal of QSL, in which a quantum field theory describes the ground state properties and excitations [3].

We give an overview and present the last developments of our work on different rare-earth pyrochlore materials with potential for QSL states. In Tb<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub>, where a sizeable gap isolates the non-Kramers ground state doublet at low temperature, a large amount of anion Frenkel disorder leads to quenched random crystal fields and disordered magnetic interactions. The detailed study of this material demonstrates that disorder can play a crucial role in preventing long-range magnetic order at low temperatures, and instead induces a strongly-fluctuating Coulomb spin liquid [4]. In Pr<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub>, another QSL candidate based on non-Kramers ions [5], we find a quasielastic structure factor with pinch points - a signature of a classical spin ice - that are partially suppressed [6], as expected in the quantum-coherent regime of the QSI lattice field theory at finite temperature [7,8]. Inelastic neutron scattering measurements also reveal magnetic excitations in this material at low temperature, which we relate to the theoretical expectations for the QSI ground state. Taken together, the suppressed pinch-points and the spectrum of magnetic excitations constitute evidence that the low-energy physics of Pr<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub> can be described by emergent quantum electrodynamics [6]. In Ce<sub>2</sub>Sn<sub>2</sub>O<sub>7</sub>, macroscopic measurements suggest an antiferromagnetic liquid ground state with quantum fluctuations [9]. We present results on Ce<sup>3+</sup> pyrochlore oxides that connect with theoretical proposals of QSL states based on dipole-octupole Kramers doublets [10,11].

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#### Multipolar order and superconductivity in Pr(TM)<sub>2</sub>(Al,Zn)<sub>20</sub> Kondo Materials

SungBin Lee (KAIST), Arun Paramekanti (University of Toronto), Frederic Freyer (University of Cologne), Jan Attig (University of Cologne), Simon Trebst (University of Cologne) and Yong Baek Kim (University of Toronto)

In heavy fermions, many exotic phenomena coexist such as hidden order, unconventional metal and superconductivity. In particular, Pr based Kondo materials Pr(TM)<sub>2</sub>(Al,Zn)<sub>20</sub> exhibit unique multipolar order and superconductivity.[1-4] Motivated by recent experimental results, we will focus on the multipolar ordering of Pr<sup>3+</sup> and discuss possible phase transitions, in addition to the field effect.[5-6] Then we will also discuss the unique feature of superconductivity driven by quadrupolar order fluctuations.

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# 0.18 Frustrated Magnetism III

Saturday, 8:30-10:00 Batista, Romhanyi, Tsvelik

#### Dynamical structure factor of the triangular Heisenberg model.

Cristian D. Batista (University of Tennessee)

Motivated by recent experiments in Ba3Co2Sb2O9, I will derive the zero temperature dynamical structure factor  $S(q,\omega)$  of the triangular lattice Heisenberg model using a Schwinger Boson approach that includes the Gaussian fluctuations (1/N correction) of the saddle point solution. While the ground state of this model exhibits a well-known 120 degree magnetic ordering, the excitation spectrum revealed by  $S(q,\omega)$  has a strong quantum character, which is not captured by low-order 1/S expansions. The low-energy magnons consist of two-spinon bound states confined by the gauge fluctuations of the auxiliary fields. This composite nature of the magnons leads to an internal structure of the magnon peaks. In addition, the continuum of high-energy spinon modes extends up to three times the single-magnon bandwidth.

#### Topological bands and multipolar edge states in quantum magnets.

Judit Romhányi (OIST)

Excitations of ordered insulating magnets gained renewed interest due to their potential to realize the nontrivial topological properties discovered for weakly interacting electron systems. Notable examples are the Weyl magnons emerging in breathing pyrochlore antiferromagnets [1] and the Haldane model realized in the magnon spectrum of ferromagnetic Fe-based honeycomb lattice [2].

In this talk we attempt to go beyond these parallels and explore what else is there in the unconventional excitations of quantum magnets. We study the topologically nontrivial multiplet excitations of anisotropic spin-1/2 antiferromagnets where the magnetic units are entangled spin clusters. We show that the excitations can be characterized by spin multiplets. Applying magnetic field we can tune the magnon modes through a band touching topological phase transition, where spin-S Dirac cones are formed by the touching of 2S+1 bands. In the topologically nontrivial regime the multiplet excitations have large Chern numbers:  $-2S, \ldots, 2S$  [3]. When the system has open boundaries we find novel quadrupolar edge states [4].

REFERENCES [1] F.-Y. Li, Y.-D. Li, Y. B. Kim, L. Balents, Y. Yu and G. Chen, Nat. Comm. **7** 12691 (2016). [2] H.-S. Kim and H.-Y. Kee, npj Quantum Materials **1** 20 (2017); [3] J. Romhányi, K. Penc and R. Ganesh Nat. Comm. **6** 6805 (2015); [4] J. Romhányi arXiv:1801.07950 (2018)

#### Chiral Spin Order in Kondo-Heisenberg systems.

A. M. Tsvelik (Brookhaven National Laboratory), O. M. Yevtushenko (Maximilian Ludwig University)

We demonstrate that Kondo-Heisenberg systems, consisting of itinerant electrons and localized magnetic moments (Kondo impurities), can be used as a principally new platform to realize chiral spin order. The underlying physics is governed by a competition of the Ruderman-Kittel-Kosuya-Yosida (RKKY) indirect exchange interaction between the local moments with the direct Heisenberg one. When the direct exchange is weak and RKKY dominates the isotropic system is in the disordered phase. A moderately large direct exchange leads to an Ising-type phase transition to the phase with chiral spin order. Our finding paves the way towards pioneering experimental realizations of the chiral spin liquid in low dimensional systems with spontaneously broken time reversal symmetry.

A. M. Tsvelik and O. M. Yevtushenko, accepted to Phys. Rev. Lett., Editors' Suggestion.

# 0.19 Triangular I

Saturday, 10:30-12:00 Chen, Mourigal, Chernyshev

#### Frustrated metal Pr<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> and spin liquid candidate YbMgGaO<sub>4</sub>.

Gang Chen (Fudan Univ)

In this talk, we discuss the frustrated metal Pr<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> and the triangular lattice spin liquid candidate YbMgGaO<sub>4</sub>. For Pr<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>, we explain the interplay between the Pr local moments and the Ir conduction electrons. It has been demonstrated experimentally that the Ir conduction electrons form a Luttinger semimetal with a quadratic band touching at Gamma point. Depending on the Ir and O contents, the Pr local moments can develop a magnetic order with a finite ordering wave vector. We consider the band structure construction of the Ir conduction in the presence of the Pr magnetic order. We predict the symmetry protected Dirac band touching as well as the topologically protected Weyl nodes. We further study the topological engineering by the external magnetic field. For YbMgGaO<sub>4</sub>, we mainly focus on our phenomenological explanation and prediction of the excitation continuum in YbMgGaO<sub>4</sub>, and this continuum is interpreted to be spinon continuum of a spinon Fermi surface spin liquid state.

#### Anomalous spin dynamics in triangular quantum magnets.

Martin Mourigal (Georgia Tech)

The spin-1/2 triangular-lattice antiferromagnet is a central model in frustrated quantum magnetism: it is the first two-dimensional magnet proposed to host a SU(2) symmetric resonating valence-bond ground-state and its fractionalized magnetic excitations. Although it is now accepted that the model, at least in its simplest Heisenberg form, orders magnetically, it remains intimately associated with the concepts of quantum spin-liquid and exotic magnetic excitations. In the last few years, advances in materials discovery, crystal growth, neutron spectroscopy and theory have fueled a lively triangular-lattice antiferromagnet "Renaissance". In this talk, I will describe recent neutron scattering investigations on two realizations of this model: the transition metal compound Ba3CoSb2O9 and the rare-earth system YbMgGaO4. Experimental results elucidate the role of quantum fluctuations and entanglement, spin-orbit coupling, chemical disorder, and non-linear effects in generating anomalous spin dynamics in these materials.

#### Topography and mimicry on a triangular lattice

Sasha Chernyshev (UCI), Zhenyue Zhu (UCI), P. A. Maksimov (UCI), Steven R. White (UCI)

There is a significant recent interest in spin systems with strongly-anisotropic frustrating spin interactions due to possible exotic ground states. We have explored an extended 3D phase diagram of a class of such models on an ideal triangular lattice using density-matrix renormalization group (DMRG) and quasiclassical approaches [1,2] and have mapped out the topography of the region that can harbor a spin liquid state. A 4D extension of this phase diagram naturally connects to a different spin liquid phase of the isotropic  $J_1$ – $J_2$  model. We find that spin-spin correlations are nearly identical between these two limits [2], making a strong case that their respective spin liquids are isomorphic to each other. For YbMgGaO<sub>4</sub>, a rare-earth-based triangular-lattice antiferromagnet with anisotropic spin-spin interactions, our analysis finds no transitions to a spin liquid near experimentally relevant range of parameters [1,2]. We have proposed that a randomization of the subleading pseudo-dipolar interactions due to spatially-fluctuating charge environment of the magnetic ions can successfully mimic a spin liquid by forming short-range stripe-ordered domains, producing the structure factor that is in agreement with experiment. This spin-liquid mimicry scenario is relevant to other quantum magnets with fragile ground states selected by an order-by-disorder fluctuations and random environments.

[1] Zhenyue Zhu, P. A. Maksimov, Steven R. White, and A. L. Chernyshev, Phys. Rev. Lett. **119**, 157201 (2017); [2] Zhenyue Zhu, P. A. Maksimov, Steven R. White, and A. L. Chernyshev, arXiv:1801.01130, (to be unpublished).

# 0.20 Triangular II

Saturday, 1:30-3:00 Starykh, Clark, Tanaka

#### Spinon resonance of two-dimensional U(1) spin liquids with Fermi surfaces

Oleg Starykh (University of Utah) and Leon Balents (KITP, UCSB)

We investigate signatures of spin liquids with spinon Fermi surfaces in electron spin resonance experiments. We focus on the magnetic field (h) and temperature (T) dependence of the linewidth  $\eta$  of the resonance peak in the ESR absorption spectrum. We show that in the presence of DM interaction, the linewidth is determined by the low-energy U(1) gauge fluctuations resulting in a characteristic  $\eta \sim h^{2/3}$  scaling at T=0 and a more complicated behavior  $\sim T/h + T^{2/3} f(h/T)$ , with an explicit form of the scaling function f(x), at finite T. We find that exchange anisotropy results in a weaker h and T dependence of  $\eta$ . We discuss relevance of our findings to experiments on the spin liquid candidate  $\kappa$ -ET and related materials.

#### Two-Dimensional Spin Liquid Behaviour in the Triangular-Honeycomb Antiferromagnet, TbInO<sub>3</sub>.

L. Clark (University of Liverpool), G. Sala (Oak Ridge National Laboratory), D. Maharaj (McMaster University), M. B. Stone (Oak Ridge National Laboratory), K. S. Knight (ISIS Neutron and Muon Facility), M. T. F. Telling (ISIS Neutron and Muon Facility), X. Wang (Rutgers University), J. Kim (Rutgers University), Y. Lee (Rutgers University), S.-W. Cheong (Rutgers University) and B. D. Gaulin (McMaster University)

Spin liquids in frustrated magnets continue to attract a wealth of theoretical and experimental interest due to their exotic emergent nature. Recently, the roles that strong spin-orbit coupling and crystal field effects may play in engineering spin liquid ground states, in both transition metal-based [1] and rare-earth magnetic materials [2], have become particularly intriguing focal points.

In this vein, we present a detailed low-temperature structural and magnetic study of TbInO<sub>3</sub> [3], which crystallises in the non-centrosymmetric hexagonal space group  $P6_3cm$  with the LuMnO<sub>3</sub>-type structure [4]. As such, TbInO<sub>3</sub> consists of quasi-two-dimensional triangular layers of Tb<sup>3+</sup> ions that reside at two distinct crystallographic sites. We show that although the system displays Curie-Weiss behaviour, with a Weiss temperature  $\theta = -17$  K, muon spectroscopy and powder neutron diffraction measurements give no evidence for long-range magnetic order to temperatures of 0.1 K and 0.46 K, respectively. Furthermore, we present time-of-flight inelastic neutron scattering data that reveal the development of short-range, two-dimensional antiferromagnetic correlations in TbInO<sub>3</sub> at  $T \sim |\theta|$ , as well as a rich spectrum of crystal field excitations arising from the Tb<sup>3+</sup> ions. This spectrum can be understood in terms of a magnetic doublet ground state at one of the two Tb<sup>3+</sup> ion sites but a non-magnetic singlet ground state at the other, with a low-lying excited state  $\sim 8$  K above the singlet ground state. At temperatures below this gap, the distorted triangular magnetic sublattice in TbInO<sub>3</sub> is thus diluted and an undistorted honeycomb network of Tb<sup>3+</sup> ions emerges. The fact that no long-range magnetic order is evident to the lowest measurable temperatures motivates our suggestion that the observed spin liquid phase of TbInO<sub>3</sub> arises from strong magnetic frustration. We consider the possible origins of this frustration, including anisotropic exchange interactions on the honeycomb lattice of Tb<sup>3+</sup> ions to form a spin liquid state akin to that predicted for honeycomb magnets with anisotropic, bond-dependent Kitaev interactions [5].

[1] A. Banerjee et al., Science, 2017, 356, 1055, [2] K. A. Ross et al., Phys. Rev. X, 2011, 1, 021002, [3] L. Clark et al., in preparation, 2018, [4] C. Pistorius and G. Kruger, J. Inorg. Nucl. Chem., 1976, 38, 1471, [5] J. Chaloupka et al., Phys. Rev. Lett., 2010, 105, 027204.

#### Structure of Magnetic Excitations in a Spin-1/2 Triangular-Lattice Heisenberg Antiferromagnet Ba<sub>3</sub>CoSb<sub>2</sub>O<sub>9</sub>

H. Tanaka (Tokyo Institute of Technology), S. Ito (Tokyo Institute of Technology), N. Kurita (Tokyo Institute of Technology), S. Ohira-Kawamura (J-PARC Center), K. Nakajima (J-PARC Center), S. Itoh (KEK), K. Kuwahara (Ibaraki University), and K. Kakurai (CROSS Tokai)

An spin-1/2 triangular-lattice Heisenberg antiferromagnet (TLHAF) is a prototypical frustrated quantum magnet, which exhibits remarkable quantum many-body effects arising from spin frustration and quantum fluctuation. The ground-state properties of an S=1/2 TLHAF are theoretically well understood. Theoretical predictions including a quantum magnetization plateau at one-third of the saturation magnetization were verified by experiments on  ${\rm Ba_3CoSb_2O_9}$ , which is considered to be the best experimental realization of the S=1/2 TLHAF [1]. However, magnetic excitations are less well understood and the theoretical consensus is limited. The experimental study of the magnetic excitations in S=1/2 TLHAFs has also been limited [2]. In this presentation, we show the whole structure of magnetic excitations in  ${\rm Ba_3CoSb_2O_9}$  investigated by inelastic neutron scattering [3]. The excitation spectra have a three-stage energy structure. The lowest first stage is composed of dispersion branches of single-magnon excitations. The second and third stages are dispersive continua. The excitation continuum extends above 10 meV, which is six times larger than the exchange

[1] Y. Shirata *et al.*, Phys. Rev. Lett. **108**, 057205; T. Susuki *et al.*, Phys. Rev. Lett. **110**, 267201 (2013).
[2] J. Ma *et al.*, Phys. Rev. Lett. **116**, 087201 (2016).
[3] S. Ito *et al.*, Nat. Commun. **8**, 235 (2017).

interaction J = 1.67 meV. This result strongly suggests that the excitation continuum in the S = 1/2 TLHAF is composed of multiple excitations of fractionalized spin excitations, even if the ground state is an ordered state.

## 0.21 Poster Session I

## Tuesday 7/10

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1. A. Akbari-Sharbaf (Université de Sherbrooke)
                       2. K. Aoyama (Osaka University)
                     3. S. Asai (ISSP. The Univ. of Tokyo)
                           4. J. Badger (UC Davis)
                       5. K. Beauvois (CEA Grenoble)
                                6. D. Bruning
                        7. C. Buhariwalla (McMaster)
                 8. H.B. Cao (Oak Ridge National Laboratory)
                           9. Tyler Cary (UC Davis)
                10. V. Cathelin (Institut Néel, Grenoble, France)
                       11. H. Changlani (Johns Hopkins)
12. E. Constable (Vienna University of Technology, Austria, Institut Néel, France)
                13. P. P. Deen (ESS, University of Copenhagen)
                            14. Z.-H. Dong(Fudan)
                 15. Zhiling Dun (Georgia Tech, U. Tennessee)
                         16. K. Povarov (ETH Zurich)
                             17. R. Edberg (KTH)
               18. M. Frontzek (Oak Ridge National Laboratory)
                            19. S. Giblin (Cardiff)
         20. K. Guratinder (LNS, PSI and Uni. of Geneva, Switzerland)
                          21. Yuya Haraguchi(ISSP)
                             22. E. A. Henriksen
                   23. G. Hester (Colorado State University)
                    24. L.J. Heyderman (ETH Zurich-PSI)
                          25. Kyusung Hwang (OSU)
                         26. K. Kamazawa (CROSS)
                           27. Y. Kamiya (RIKEN)
                         28. H. Koushiro (Osaka Uni.)
                          29. A. Koga (Tokyo Tech.)
                    30. N. Kurita (Tokyo Inst. Tech., Japan)
            31. D. Lançon (ETH Zurich-Paul Scherrer Institute, CH)
                     32. K. Matsuhira (Kyushu Inst. Tech.)
                33. C. Mauws (Univ. Winnipeg, Univ. Manitoba)
                    34. T. Müller (University of Wurzburg)
                      35. O. Mustonen (Aalto University)
                       36. C. Paulsen (CNRS Grenoble)
                         37. J. Reid (U. of Waterloo)
                             38. K. A. Ross (CSU)
                    39. M. Saito (Tokyo Institute of Tech.)
                    40. G. Simutis (Paul Scherrer Institute)
              41. M. Tabata (Dept. Phys, Aoyama Gakuin Univ.)
                        42. H. Tomishige (Tokyo Tech)
                       43. A. Turrini (PSI, UniGeneva),
                   44. K. Tustain (University of Liverpool)
                      45. M. Udagawa (Gakushuin Univ.)
                       46. Christopher N. Varney(UWF)
                          47. O. Young (HFML, NL)
               48. M. Zŭković (P.J. Sáfárik University, Slovakia)
                        49. L. Shu (Fudan University)
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# Tunable magnetic phase from antiferromagnetic order to quantum spin liquid in the 1/6th-filled breathing kagome lattice.

A. Akbari-Sharbaf (Université de Sherbrooke), R. Sinclair (University of Tennessee), A. Verrier (Université de Sherbrooke), D. Ziat (Université de Sherbrooke), H. D. Zhou (University of Tennessee), X. F. Sun (University of Science and Technology of China), J. A. Quilliam (Université de Sherbrooke)

One of the most sought after magnetic phases is the quantum spin liquid (QSL), whereby spins form a highly-entangled quantum ground state that supports fractional excitations. We will present results on a family of compounds  $\text{Li}_2\text{In}_{1-x}\text{Sc}_x\text{Mo}_3\text{O}_8$  (x=0.2,0.4,0.6,0.8,1) which allows us to tune the magnetic ground state from antiferromagnetic order to QSL [1]. The crystal structure for this family can be viewed as Mo ions arranged on a breathing kagome lattice with two distinct Mo-Mo bond lengths. The Mo magnetic planes are separated by nonmagnetic layers composed of Li, In, and Sc ions. XRD reveals the breathing parameter  $\lambda$ , defined as the ratio of long to short Mo-Mo bond length, changes non-monotonically with increasing Sc concentration x, where  $\lambda$  is a minimum for x=0.6 for this series. The magnetic ground state for this family, deduced by muon spin rotation, is correlated with the breathing parameter, where small  $\lambda$  favours a QSL phase, while large  $\lambda$  favours antiferromagnetic order. Magnetic susceptibility for the sample with a pure QSL phase (namely x=0.6) displays an anomaly previously reported for the QSL candidate LiZn<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>, whereby the Curie constant is reduced by a factor of three below a crossover temperature [2]. Our experimental results are consistent with the theoretical framework developed by Chen *et al.* based on an extended Hubbard model for a 1/6th filled breathing kagome lattice [3]. We attributed the QSL phase in our samples to a cluster Mott insulating phase with a novel plaquette charge order predicted by their model.

[1] A. Akbari-Sharbaf, R. Sinclair, A. Verrier, D. Ziat, H.D. Zhou, X. F. Sun, and J.A. Quilliam, Tunable quantum spin liquidity in the 1/6th-filled breathing kagome lattice. arXiv preprint arXiv:1709.01904 (2017). (submitted to Phys. Rev. Lett.); [2] J.P. Sheckelton, J.R. Neilson, D.G. Soltan, and T.M. McQueen, Possible valence-bond condensation in the frustrated cluster magnet LiZn 2 Mo 3 O 8, Nature Materials 11, 493 (2012); [3] G. Chen, H.Y. Kee, and Y.B. Kim. Cluster Mott insulators and two Curie-Weiss regimes on an anisotropic kagome lattice, Phys. Rev. B, 93: 245134 (2016).

## Effects of local lattice distortions on the spin ordering in Heisenberg antiferromagnets on breathing pyrochlore lattices

K. Aoyama and H. Kawamura (Osaka University)

Antiferromagnets on the pyrochlore lattice are typical examples of frustrated magnets. It has been theoretically established that with the nearest-neighbor (NN) antiferromagnetic interaction alone, classical Heisenberg spins on the pyrochlore lattice do not order at any finite temperatures due to the massive degeneracy of the ground state. Weak perturbative interactions such as further-neighbor interactions would lift the degeneracy, eventually leading to the magnetic ordering, but the mechanism of the degeneracy lifting generally depends on specific materials. In the spinel oxides ACr<sub>2</sub>O<sub>4</sub> (A=Zn, Cd, Hg, Mg), where the magnetic ion Cr<sup>3+</sup> with S=3/2 forms the pyrochlore lattice, the system undergoes a first-order transition into the magnetic long-range-ordered state accompanied by a simultaneous structural transition which lowers the crystal symmetry. This suggests that the spin-lattice-coupling (SLC) is essential in this class of antiferromagnets. Recently, a new type of the pyrochlore lattice, so-called breathing pyrochlore lattice, has been realized in the chromium oxides, LiGaCr<sub>4</sub>O<sub>8</sub> and LiInCr<sub>4</sub>O<sub>8</sub> [1]. This lattice consists of an alternating array of small and large tetrahedra, and thus, the NN interactions on the small and large tetrahedra, *J* and *J'*, can take different values. In these compounds, the magnetostructural transition similar to that in ACr<sub>2</sub>O<sub>4</sub> has been also observed. In view of such an experimental situation, we theoretically investigate SLC effects in the classical Heisenberg model on breathing pyrochlore lattices.

We have studied lattice distortion effects on the spin ordering based on the so-called site phonon model. For the uniform pyrochlore lattice, the SLC originating from site phonons induces a first-order transition into two different types of collinear magnetic ordered states. The state realized at stronger SLC is cubic symmetric characterized by the magnetic  $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$  Bragg peaks, while that at weaker SLC is tetragonal symmetric characterized by the (1,1,0) ones, each accompanied by the commensurate local lattice distortions [2]. In this study, we apply the site phonon model to the breathing pyrochlore antiferromagnets, and examine effects of the breathing lattice structure, namely, the ratio J'/J, on the spin-lattice-coupled orderings. Our Monte Carlo simulations show that the (1,1,0) state is robust against J'/J and its magnetic structure is the same as that in the AFM phase of LiInCr<sub>4</sub>O<sub>8</sub> [3], suggesting that this compound is in the

weaker SLC regime. On the other hand, in the stronger SLC regime which is not yet achieved experimentally, the  $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$  state has three different ordering patterns (type I, II, and III) depending on the value of J'/J. In contrast to the type I order appearing in the uniform case, the type II and III orders are peculiar to the breathing pyrochlore lattices and have non-cubic magnetic structures. We demonstrate that the difference in the ordering patterns of the three  $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$  phases is reflected in the residual entropy. In the presentation, we will also discuss magnetic field effects on the spin-lattice-coupled orders.

[1] Y. Okamoto, G. J. Nilsen, J. P. Attfield, and Z. Hiroi, Phys. Rev. Lett. 110, 097203 (2013).
[2] K. Aoyama and H. Kawamura, Phys. Rev. Lett. 116, 257201 (2016).
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# Neutron Scattering study on Spin-Density-Wave State in Magnetic Field for S=1/2 One-dimensional Frustrated Chain Compound NaCuMoO<sub>4</sub>(OH).

S. Asai (ISSP. The Univ. of Tokyo), T. Oyama (ISSP. The Univ. of Tokyo), A. Nakao (CROSS), K. Munakata (CROSS), K. Nawa (IMRAM, Tohoku Univ.), Z. Hiroi (ISSP. The Univ. of Tokyo), and T. Masuda (ISSP. The Univ. of Tokyo)

In S = 1/2 one-dimensional frustrated chain with nearest-neighbor ferromagnetic interaction  $J_1$  and next-nearest-neighbor antiferromagnetic interaction  $J_2$ , the ground state exhibits various quantum phases depending on the ratio of  $J_1$  to  $J_2$  [1]. Theoretical study predicted that applying magnetic field induces unconventional magnetic states such as the spin multipole order in the vicinity of the saturation field [2]. NaCuMoO<sub>4</sub>(OH) is an experimental realization of the system having decent energy scale for the magnetic interactions [3]. Our recent neutron diffraction study at zero field indicates that the proper-screw magnetic structure is realized below 0.6 K [4]. When the magnetic field is applied, the transition to the spin-density-wave (SDW) state is theoretically predicted [2]. Recent NMR and heat capacity study indicated the SDW phase at H > 1.5 T. [5]. In order to investigate the magnetic state, we carried out a neuron diffraction experiment on the single crystal in the magnetic field. We observed the magnetic Bragg peak at  $(0, \delta, 0)$  ( $\delta \sim 0.48$ ) in zero field, which is consistent with the previous result. The value of  $\delta$  is independent of the field below 1 T. Meanwhile, it decreases with increasing the field above 2.5 T. This behavior is consistent with the theoretical prediction for the SDW<sub>2</sub> state in the frustrated ferromagnetic chain [6].

REFERENCES.[1] S. Furukawa *et al.*, Phys. Rev. Lett. **105**, 257205 (2010). [2] T. Hikihara *et al.*, Phys. Rev. B **78**, 144404 (2008). [3] K. Nawa *et al.*, J. Phys. Soc. Jpn. **83**, 103702 (2014). [4] S. Asai *et al.*, 2016 JPS Autumn meeting 14pBK-3. [5] K. Nawa *et al.*, Phys. Rev. B **96**, 174433 (2017). [6] M. Sato *et al.*, Phys. Rev. B **79**, 060406 (2009).

## Antiferromagnetic Ordering Competition in Nd-doped $CeIn_3$ .

J. Badger, P. Klavins, and V. Taufour

Both CeIn $_3$  and NdIn $_3$  crystallize in the same cubic structure  $(Pm\overline{3}m)$  and show antiferromagnetic ordering below  $10.1~\rm K$  and  $5.9~\rm K$ , respectively. We investigate the magnetic ordering of single crystals of Ce $_{1-x}\rm Nd_x$ In $_3$  and discover a region of frustrated magnetism near  $x\sim0.3$  where the magnetic order is suppressed to below  $1.8~\rm K$ . In this region, the two antiferromagnetic orders appears to be in competition with one another despite that fact that antiferromagnetic interactions are still observed. We present the sample synthesis, and characterizations, as well as a discussion of the observed magnetic properties in the context of heavy-fermion behavior, percolation of magnetic ordering, and magnetic anisotropy.

## Magnetic interactions in the frustrated pentagonal compound Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub>

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The Fe<sup>3+</sup> ions in Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub> materialize the first analogue of a magnetic pentagonal lattice [1]. The unit cell contains two different sites of four iron atoms each, which have different connectivities with the other irons (three or four neighbours for Fe<sub>1</sub> and Fe<sub>2</sub> respectively), and that form a lattice of pentagons. Because of its odd number of bonds per elemental brick, this lattice is prone to geometric frustration. The compound magnetically orders around 240 K: the resulting spin configuration on the two sites is the same, i.e. two orthogonal pairs of antiferromagnetic spins in a plane, with a global rotation between the two sites Fe<sub>1</sub> and Fe<sub>2</sub>. This peculiar magnetic structure, which is the result of the complex connectivity, has opened new perspectives in the field of magnetic frustration.

Here, we present the work in progress concerning the understanding and the consequences of the peculiar magnetic interactions in this original system. First, magnetization distribution maps have been measured at the Institut Laue Langevin (ILL) using polarized neutrons under an applied magnetic field. Remarkably, the magnetic moments of the Fe<sub>1</sub> sites, contrary to those of Fe<sub>2</sub>, are extremely weakly (or even not) polarized by the field both in the paramagnetic phase and in the ordered one. This indicates a paramagnetic liquid of classical spin dimers that condensate into a long-range arrangement below the Néel temperature. These dimers are stabilized by a strong antiferromagnetic coupling between pairs of Fe<sub>1</sub> atoms combined with a high degree of frustration. In a second step, the magnetic excitations have been investigated by inelastic neutron scattering using triple axis spectrometers at the LLB and the ILL. The confrontation of the experimental results with spinwave calculations confirms the hierarchy of the interactions between the iron sites in the lattice, and therefore the validity of the classical spin dimer picture.

In addition, we also report the evolution of the magnetic structure of Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub> under isostatic pressure (from 0 to 10 GPa) from powder neutron diffraction experiments performed at the ILL. At room temperature, we confirm the presence of a structural phase transition observed at approximatively 6.89(6) GPa by X-Ray diffraction and Raman spectroscopy [2]. From the low temperature patterns, we find, using Rietveld refinements, a magnetic transition at this pressure toward a new magnetic arrangement that we discuss with respect to magnetic frustration.

Our new experimental results on Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub> open interesting perspectives in the field of frustrated pentagonal lattices.

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## Residual entropy and monopole heat transport in dilute spin ice $(Dy_{1-x}Y_x)_2Ti_2O_7$ .

D. Brüning, S. Scharffe, J.-F. Welter, G. Kolland, and T. Lorenz —

The spin ice  $\mathrm{Dy_2Ti_2O_7}$  is a geometrically frustrated spin system of corner-sharing tetrahedra with a strong Ising anisotropy of the Dy spins. Thus, spins can only point into or out of each tetrahedron yielding a 2in-2out ground state. The lowest excitation is a single spin flip which creates a pair of 1in-3out and 3in-1out configurations on neighboring tetrahedra. Such a pair can fractionalize into two individual excitations, namely magnetic monopoles, that can propagate almost independently within the pyrochlore lattice. The entropy of  $\mathrm{Dy_2Ti_2O_7}$  reveals a plateau-like feature close to Pauling's residual entropy around 0.5 K derived originally for water ice. Ultraslow thermal equilibration prevents an unambiguous determination towards lower temperature. We analyze the influence of non-magnetic yttrium dilution on the low-temperature entropy of  $(\mathrm{Dy_{1-}}_x Y_x)_2 \mathrm{Ti_2O_7}$ . The ultraslow thermal equilibration rapidly vanishes with increasing x, the low-temperature entropy systematically decreases, and its temperature dependence strongly increases. Our data reveals a non-degenerate ground state for  $x \geq 0.1$  that is compared to different theoretical approaches. Additionally, we present heat transport data of the dilution series where we extract a magnetic contribution  $\kappa_{\mathrm{mag}}$  to the total heat transport and discuss the role of magnetic monopoles.

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## Correlations in Ferromagnetic Titanate Pyrochlores as Revealed by SANS.

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We have carried out small angle neutron scattering measurements on single crystals of two pyrochlores that display ferromagnetic Curie-Weiss susceptibilities,  $Yb_2Ti_2O_7$  and  $Ho_2Ti_2O_7$ .  $Ho_2Ti_2O_7$  is established as displaying a prototypical classical dipolar spin ice ground state, while Yb2Ti2O7 has been purported as a candidate for a quantum spin ice ground state. Our results for  $Yb_2Ti_2O_7$  show distinct SANS features below its  $\Theta_{CW}$  (0.50 K), with rods of diffuse scattering along 111 directions, off-rod scattering which peaks in temperature near  $\Theta_{CW}$ , and quasi-Bragg scattering at very small angles which correlates well with the measured  $T_C$  of 0.26 K. The quasi-Bragg scattering corresponds to finite extent ferromagnetic domains approximately 140 Å across, at the lowest temperatures. We interpret the 111 rods of diffuse scattering as arising from domain boundaries between the finite-extent ferromagnetic domains. In contrast the SANS signal in  $Ho_2Ti_2O_7$  is isotropic within the (HHL) plane around Q=0. However the strength of this overall SANS signal has a temperature dependence resembling that of the magnetic heat capacity, with a peak near 3 K. Below the break between the field-cooled and the zero-field cooled susceptibility in  $Ho_2Ti_2O_7$  near 0.60 K, the SANS signal is very low, approaching zero.

## Diffuse scattering in a 2D square magnet\*

H.B. Cao (Oak Ridge National Laboratory), Y. H. Liu (Oak Ridge National Laboratory), A. S. Admasu (Rutgers University), J. W. Kim (Rutgers University) and S.-W. Cheong (Rutgers University)

A two dimensional (2D) rare earth magnet  $Tb_2SrAl_2O_7$  was investigated by neutron diffuse scattering at Correli at SNS and HB3A at HFIR, at ORNL. A "spin-ice" like diffuse scattering pattern was observed in the HK-scattering plane and rod-shape diffuse scattering along the L indicates its 2D magnet feature. The results agree with the magnetic measurements that show no magnetic order down to 1.8 K. The experimental details and data modeling on this new 2D "spin-ice" system will be presented.

\* This research used resources at the Spallation Neutron Source and the High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

## Tricriticality in crossed Ising chains.

Tyler Cary (UC Davis), Rajiv Singh (UC Davis) and Richard Scalettar (UC Davis)

We explore the phase diagram of Ising spins on one-dimensional chains that criss-cross in two perpendicular directions and that are connected by interchain couplings. This system is of interest as a simpler, classical analog of a quantum Hamiltonian that has been proposed as a model of magnetic behavior in  $Nb_{12}O_{29}$  and also, conceptually, as a geometry that is intermediate between one and two dimensions. Using mean-field theory as well as Metropolis Monte Carlo and Wang-Landau simulations, we locate quantitatively the boundaries of four ordered phases. Each becomes an effective Ising model with unique effective couplings at large interchain coupling. Away from this limit, we demonstrate nontrivial critical behavior, including tricritical points that separate first- and second-order phase transitions. Finally, we present evidence that this model belongs to the two-dimensional Ising universality class.

## Spin dynamics in pyrochlore iridates $Ho_2Ir_2O_7$ and $Dy_2Ir_2O_7$ .

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Pyrochlore iridate oxides are materials of formula  $R_2 Ir_2 O_7$ . In these compounds, the iridium and rare-earth (R) ions lie on two interpenetrated pyrochlore lattices. For most of the rare-earth ions, the iridium sublattice orders in an all-in all-out magnetic arrangement at about 100 K, and generates a molecular field oriented along the local  $\langle 111 \rangle$  directions on the rare-earth sublattice [1]. When R=Ho or Dy, this staggered magnetic field competes at very low temperature with the R-R ferromagnetic interactions.

We have shown that in  $\mathrm{Ho_2Ir_2O_7}$  this competition results in magnetic fragmentation, a recently discovered phase in which the magnetic moments fragment, leading to the superposition of a magnetically ordered phase and a persistently fluctuating one [2]. It manifests as the coexistence of spin-ice diffuse scattering with an all-in all-out ordering, whose ordered magnetic moment is half of the total moment. From this phase are emerging excitations, magnetic monopoles, which evolve in a periodic potential, induced by the iridium sublattice. It gives rise to unconventional dynamics that differ from canonical spin ice.

In my talk, I will show that  $\mathrm{Dy_2Ir_2O_7}$  also stabilizes a fragmented phase. I will focus on the slow dynamics at very low temperature measured by ac susceptibility between 50 mK and 4 K. Indeed, relaxation times can be described with an Arrhenius law in both systems but with different time scales and energy barriers. I will eventually compare these results with the dynamics of classical spin ices.

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## The mother of all states of the kagome quantum antiferromagnet.

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Frustrated quantum magnets are a central theme in condensed matter physics due to the richness of their phase diagrams. They support a panoply of phases including various ordered states and topological phases. We report an exactly solvable macroscopically degenerate point in the XXZ model on the spin-1/2 kagome quantum antiferromagnet, for the ratio of Ising to transverse coupling  $J_z/J=-1/2$  [1]. This point has "three-color" wavefunctions as its exact ground states and is proximate to many competing phases, explaining the source of the complexity of the phase diagram. We identified five phases near this "mother" point, including spin-liquid and broken-symmetry phases. Extending the central ideas, we have also recently developed an exact map between the more familiar topological and localized magnons on the kagome lattice and three quantum coloring wavefunctions [2]. Using this map we show that the  $J_z/J=-1/2$  point is a critical point for several magnetization sectors.

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# Spin-lattice coupling and vibronic processes in the quantum spin ice candidate Tb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> probed by THz spectroscopy

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In the study of geometrically frustrated magnetism, the precise nature of the ground state in Tb2Ti2O7 has remained a long-standing conundrum. In this pyrochlore material, no conventional spin-ice or long-range magnetic order is stabilized, even at very low temperatures. Quantum fluctuations are suspected of being at the origin of an exotic phase, yet so far they have lacked conclusive evidence. Using high-resolution synchrotron-based terahertz spectroscopy, we

have probed the lowest energy excitations of Tb2Ti2O7. It is revealed that a double hybridization of crystal-field-phonon modes is present across a broad temperature range. This so called vibronic process affects the electronic ground state that can no longer be described solely by electronic wave functions. Rather, a collective state prevails, built on the ground and first excited crystal-field states mixed with two different phonon modes. This provides a crucial path for quantum spin-flip fluctuations to inhibit the stabilization of conventional magnetic states. The study is further complimented by recent ultrafast terahertz-pump/optical-probe measurements on the ELBE free electron laser that confirm the presence of the vibronic coupling.

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#### Dynamic signatures of the directorate state on 3D hyperkagome compounds.

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Geometrically frustrated compounds have received much interest in recent years. Examples include spin liquids[1], magnetic monopoles in spin ice[2], and the development of protected degrees of freedom[3]. Another recent example is the discovery of hidden long range multipolar order in Gadolinium Gallium Garnet, Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> (GGG)5. GGG is the archetypical example of a frustrated antiferromagnet on the hyperkagome lattice, consisting of corner-sharing triangles in an intricate pattern. The long range hidden order, a directorate state, is derived from multipoles formed from 10-spin loops and is a consequence of the interplay between antiferromagnetic spin correlations and local magnetic anisotropy. In order to determine the ubiquity of this directorate state, studies on the isostructural compound Gd<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> (GAG) have been performed and also reveal the directorate state normalised by exchange energies [6]. In order to fully understand a phenomena it is then of great importance to determine the dynamic signatures. AC susceptibility, cold inelastic neutron scattering and neutron backscattering have been performed to elucidate the dynamic signature of the directorate phase over micro to picoseconds. In the directorate phase AC susceptibility reveal distinct spin dynamics with microsecond and picosecond timescales. Inelastic neutron scattering reveal almost dispersionless spin-wave excitations, as its lowest lying excitations, and the energy of these bands of excitations can be controlled and reduced to zero through an applied field [7]. Neutron backscattering, accessing nanosecond timescales, reveals Q-independent relaxational dynamics with increasing lifetimes as the temperature is decreased and the directorate phase takes hold. An overview of these unusual dynamics is presented and assigned to the interplay between looped structures and individual spins in 3D hyperkagome compounds.

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# Quantum phase diagram and quantum Monte carlo study of the XYZ spin model: the dipole-octupole doublets on a triangular lattice.

Z.-H. Dong(Fudan), Z.-Y. Dong(Fudan), Y.-B. Yang(Fudan), X.-F. Zhang(Kaiserslautern) and G. Chen(Fudan) — Motivated by the recent activities on the geometrically frustrated rare-earth magnets, we study the quantum phase diagram of the XYZ spin model that describes the dipole-octupole doublets on a triangular lattice. Due to the absence of the sign problem of this model in a large parameter regime, we carry out the first quantum Monte carlo calculation with the stochastic series expansion method and obtain the magnetic ground states with and without the external magnetic fields. The combination of the geometrical frustration and the anisotropic spin interaction leads to a rather rich phase

diagram with a multitude of symmetry breaking orders. Moreover, the multipolar nature of the dipole-octupole doublet brings new ingredients for the quantum fluctuations in the ordered phases. The experimental relevance to the rare-earth triangular lattice materials is discussed.

## Structural and magnetic properties of the tripod kagome lattice family R3Mg2Sb3O14: a bird's eye view.

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The tripod kagome lattice R<sub>3</sub>Mg<sub>2</sub>Sb<sub>3</sub>O<sub>14</sub> (R = rare earth elements) is a recently discovered compound family that is achieved by partial ion substitutions in the pyrochlore lattice [1]. It features well isolated 2D kagome lattices with distinct tripod-like local axes. Similar to the pyrochlore lattices, a large set of rare earth spins lead to different spin anisotropies (Ising, Heisenberg, XY). Meanwhile, the symmetry reduction from 3D to 2D introduces interesting variations of the crystal electric fields, g-tensors, and spin-spin interactions, bringing up new emergent phenomenons and various of magnetic ground states [2-3]. By combing susceptibility, specific heat, neutron, and X-ray scattering measurements, our results provides a bird's eye view of the basic structural and magnetic properties of the whole family. Our recent experimental observations in two XY systems, Er<sub>3</sub>Mg<sub>2</sub>Sb<sub>3</sub>O<sub>14</sub> and Yb<sub>3</sub>Mg<sub>2</sub>Sb<sub>3</sub>O<sub>14</sub>, will also be introduced. REFERENCES. [1] Z. L. Dun, J. Trinh, K. Li, M. Lee, K. W. Chen, R. Baumbach, Y. F. Hu, Y. X. Wang, E. S. Choi, B. S. Shastry, A. P. Ramirez, and H. D. Zhou, "Magnetic Ground States of the Rare-Earth Tripod Kagome Lattice Mg<sub>2</sub>RE<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub> (RE = Gd, Dy, Er)", Phys. Rev. Lett. 116, 157201 (2016). [2] Z. L. Dun, J. Trinh, M. Lee, E. S. Choi, K. Li, Y. F. Hu, Y. X. Wang, N. Blanc, A. P. Ramirez, H. D. Zhou, "Structural and magnetic properties of two branches of the tripod-kagome-lattice family A<sub>2</sub>R<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>4 (A= Mg, Zn; R= Pr, Nd, Gd, Tb, Dy, Ho, Er, Yb)", Phys. Rev. B 95, 104439 (2017). [3] Z. L. Dun, X. Bai, J. A. M. Paddison, C. D. Cruz, M. B. Stone, T. Hong, N. P. Butch, M. Mourigal, H. D. Zhou, "Quantum dynamics in kagome ice Ho3Mg<sub>2</sub>Sb<sub>3</sub>O<sub>14</sub>", Submitted (2017).

## Strongly frustrated anisotropic spin chain Linarite PbCuSO<sub>4</sub>(OH)<sub>2</sub> in tilted magnetic fields.

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A natural mineral Linarite PbCuSO<sub>4</sub>(OH)<sub>2</sub> was recently recognized as a model S=1/2 strongly frustrated  $J_1-J_2$  spin chain material [1]. However, its magnetic phase diagram below  $T_N\simeq 2.7$  K was clearly indicating the importance of the anisotropic interactions. While the field applied along the chain direction was producing five different ordered and metastable phases including the most intriguing high field one (believed to be a spin density wave), only the slowly saturating spin spiral was found for the orthogonal field orientation [1,2].

Here we report the  $\mathbf{H}-T$  phase diagram of Linarite in tilted magnetic fields up to 10 T and temperatures down to 0.2 K. By means of torque magnetometry we investigate the phase diagram evolution as the magnetic field undergoes rotation in ba and bc planes. The key finding is the robustness of the high field spin density wave phase, which persists almost until the external field goes orthogonal to the chain direction b. In contrast, the intermediate collinear antiferromagnetic phase collapses at moderate deflection angles with respect to b axis. These findings are in line with the recently proposed anisotropic mean field model, explaining many peculiarities of magnetism in Linarite [3]. As the biaxial anisotropy is an essential ingredient for occurrence of the unusual phases in the quasi-critical  $J_1 - J_2$  spin chain, the present results are surely of importance for detailed verification of the magnetic Hamiltonian parameters of this intriguing material. [1] Willenberg  $et\ al$ ., Phys. Rev. Lett. **116** 047202 (2016); [2] Povarov  $et\ al$ ., Phys. Rev. B **94** 214409 (2016); [3] Cemal  $et\ al$ ., arXiv:1707.08051 [cond-mat.str-el] (2017)

#### Dipolar spin ice under uni-axial pressure: a Monte Carlo study

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We consider the influence of uni-axial pressure on a classical spin ice system by means of Monte-Carlo simulations. Pressure is an important probe of geometrically frustrated systems since lattice distortions tend to lift the degeneracy of the ground state, and can significantly affect the ordering tendencies of the systems. While previous studies have focused on the effects of pressure on the nearest-neighbor spin-ice model, we consider a dipolar spin-ice model relevant for the classical spin-ice material  $Dy_2Ti_2O_7$ , in which both exchange and dipolar interactions are present. In particular, we

investigate how compression inducing demagnetizing effects, affects the dipolar interaction and alters the nature of the pressure induced ordering transition.

## Magnetic properties and structure as a function of hole doping and disorder in $Pr_{2-x}Sr_xNiO_{4+\delta}$ .

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The Ruddlesden Popper phase  $\Pr_{2-x} \operatorname{Sr}_x \operatorname{NiO}_{4+\delta}$  ( $\delta=0\dots0.25$ ) has received considerable interest as material for solid oxide fuel cells due to it's ability to intercalate oxygen and a high oxygen diffusion rate. On the electronic side, it's closeness to the superconducting  $\operatorname{La}_{2-x} \operatorname{Sr}_x \operatorname{CuO}_{4+\delta}$  makes it an interesting object to investigate the magnetism as an image of the electronic properties in these systems. The undoped  $\operatorname{Pr}_2\operatorname{NiO}_4$  is a commensurate insulating antiferromagnet with  $T_N=325$  K [1, 2]. Hole doping either through Sr-doping on the Pr-site or through additional oxygen intercalation leads to the suppression of the commensurate antiferromagnetic order. The suppression is likely connected to the electronic phase separation in these systems which show up as stripe-order of  $\operatorname{Ni}^{2+}/\operatorname{Ni}^{3+}$  at higher doping concentrations [3]. In the Sr-doped case the ions are statistically distributed on the Pr-sites thus creating disorder. In the x = 0.5 case, this leads to the breakdown of the long-range magnetic order and only 2-dimensional (in-plane) correlations are observed. In contrast, the isoelectronic oxygenated compound exhibits inherent order through a superstructure formation from the intercalated oxygen ions. The resulting oxygen superstructures are different for different intercalated oxygen contents, but widths of the reflections are similar to the main lattice reflections indicating a well ordered structure through a large volume. The resulting magnetic structures at low temperatures are a superposition of 2-dimensional order and long range order. Therefore, the system  $\operatorname{Pr}_{2-x}\operatorname{Sr}_x\operatorname{NiO}_{4+\delta}$  offers the unique possibility to study the influence of order/disorder on the electronic properties of materials.

In our contribution we will present a detailed single crystal neutron diffraction study (DMC@SINQ) of three compounds from the series  $Pr_{2-x}Sr_xNiO_{4+\delta}$  comparing the fully oxygenated  $\delta=0.25$  with the isoelectronic Sr-doped compound with x=0.5. Additionally, the magnetic structure of the half oxygenated compound with  $\delta=0.12$ , which still exhibits commensurate long-range order is compared.

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## Probing the equilibrium state in frozen spin ice.

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Measurements of spin correlations by diffuse neutron scattering is one of the foremost methods of constraining the Hamiltonian of spin ice. A Recent investigation of spin ice has highlighted the possibility of very slow equilibration[1] at low temperature and/or structural defects[2] in  $Dy_2Ti_2O_7$ , leading to an absence of the Pauling entropy. Here we report on our recent investigation, to measure with neutron scattering, a sample of isotopically enriched  $^{162}Dy_2Ti_2O_7$  where the spin bath has reached equilibrium. The relaxation time is defined by specific heat[1] and susceptibility[3] measurements. The phonon bath temperature was measured using standard thermometry techniques and the spin bath temperature was measured in-situ, during the neutron scattering experiment using a small a.c. susceptometer. This allows accurate monitoring of the spin bath during the equilibration period and the measurement itself. We have performed investigations in the temperature range 0.35 - 1.1 K to allow the developed spin ice state to be examined. A theoretical calculation matches the zone-boundary scattering enabling an accurate description of  $^{162}Dy_2Ti_2O_7$  over the entire temperature range studied. To understand the origins of the relaxation mechanisms, specific heat measurements in isotopically enriched  $Dy_2Ti_2O_7$  (using  $^{162}Dy$  ions,  $^{163}Dy$  ions and a natural abundance) are also reported.

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## Quest for quantum Heisenberg AFM in spinel chalcogenides $CdYb_2X_4(X = S \text{ or } Se)$ .

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The geometrically frustrated magnetic pyrochlore lattice with exotic magnetic behaviour is well established in titanates R<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> (R= rare earth) [1]. Spinel compounds AR<sub>2</sub>X<sub>4</sub> with R-ions also residing on the pyrochlore lattice similarly exhibit unconventional magnetism [2, 4, 6]. The basic distinction between the two families is the local environment of the rare earth ions [4, 5]. Here, we present a study of crystal electric level (CEF) scheme, magnetic ground state, dynamics and their evolution with applied magnetic field of the Yb-representatives of chalcogenide spinels CdYb<sub>2</sub>X<sub>4</sub> (X= S, Se), using neutron scattering techniques. Extending recent studies on CdYb<sub>2</sub>X<sub>4</sub> [2, 3], our results illustrate and discuss both the ground state CEF level and magnetic ground state specified by k=0 propagation vector. Additionally, we observed low energy spin excitations evolving with temperature and magnetic field. This grants a possibility to identify the exchange Hamiltonian of this Heisenberg AFM with strong quantum character.

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#### Successive phase transitions in the maple-leaf lattice antiferromagnet MgMn<sub>3</sub>O<sub>7</sub>·3H<sub>2</sub>O

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The triangular lattice and its depleted lattices provide us with playgrounds for studying frustration physics in two dimension. There are two simple depletion patterns. One is the kagomé lattice with 1/4-depletion, and the other is a maple-leaf lattice with 1/7-depletion. Each site of the maple-leaf lattice has the magnetic connectivity z=5, which lies between those of the triangular and kagomé lattices, z=6 and 4, respectively. Thus, the maple-leaf lattice antiferromagnet is expected to have intermediate frustration, but has not yet been studied because of the lack of model compounds.

We present here the physical properties of the novel maple-leaf lattice antiferromagnet MgMn<sub>3</sub>O<sub>7</sub>·3H<sub>2</sub>O synthesized via a hydrothermal reaction. The compound has an isomorphic structure of the minerals Chalcophanite, ZnMn<sub>3</sub>O<sub>7</sub>·3H<sub>2</sub>O, and Ernienickelite, NiMn<sub>3</sub>O<sub>7</sub>·3H<sub>2</sub>O. The Weiss temperature is about -60 K, indicating that the magnetic interactions are dominantly antiferromagnetic among Mn<sup>4+</sup> (S=3/2) spins. Static susceptibility measurements show successive phase transitions at  $T_{N1}=5$  K and  $T_{N2}=15$  K. Moreover, the isothermal magnetization curve up to 60 T at 1.3 K shows successive magnetic-field-induced phase transitions. We will discuss the magnetic interactions and the observed successive phase transitions of MgMn<sub>3</sub>O<sub>7</sub>·3H<sub>2</sub>O based on the structural consideration from the view point of the spin frustration.

## Magnetic fluctuations in $\alpha$ -RuCl<sub>3</sub> seen by proximity effect in van der Waals heterostructures.

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Recently, the layered antiferromagnetic Mott insulator  $\alpha$ -RuCl<sub>3</sub> has been studied in bulk crystals and found to be proximate to a Kitaev quantum spin liquid. Since the QSL is primarily a two-dimensional phenomenon, it may be possible to stabilize the QSL phase in thin exfoliated samples. We have exfoliated  $\alpha$ -RuCl<sub>3</sub> to single- and few-layer flakes and studied them via Raman spectroscopy and electronic transport; the flakes are stable in air and show a structural distortion in the thinnest layers. To access the dynamics of a possible spin liquid, we have fabricated heterostructures of  $\alpha$ -RuCl<sub>3</sub> flakes layered on top of graphene Hall bars and studied variations in the well-known electronic transport of graphene. We find clear non-monotonic variations in the graphene sheet resistivity that are reproducible across several devices and consistent with the magnetic fluctuations previously seen in bulk  $\alpha$ -RuCl<sub>3</sub> by

Raman spectroscopy, neutron scattering, and numerous other experimental approaches. We thus demonstrate a new route toward exploring quantum magnetic phases that may lead toward devices based on such phenomena.

## Discovery of a New Quantum Dimer Magnet on a Strongly Spin-Orbit Coupled Honeycomb Lattice: Yb2Si2O7.

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Through the study of quantum spin liquids and high-temperature superconductivity several novel phases of matter have been discovered. One such state is the quantum dimer magnet, which, for isotropic or XXZ couplings, exhibits a field-induced antiferromagnetic phase which behaves like a Bose-Einstein condensate (BEC), and occupies a symmetric dome in the field vs. temperature phase diagram. Many compounds based on 3d magnetic cations (Cu²+, Ni²+) have been found that exhibit a quantum dimer state with a BEC phase [1]. We have found a new realization of a quantum dimer magnet based on the strongly spin-orbit coupled ion Yb³+ in the distorted honeycomb-lattice material Yb₂Si₂O7. The high spin-orbit coupling of Yb³+, combined with crystal field effects, results in pseudo-spin 1/2 angular momentum that often leads to anisotropic exchange interactions between quantum spins. Our single crystal inelastic neutron scattering, specific heat, magnetometry and ultrasound velocity measurements show the expected field-induced transition to a BEC-like magnetically ordered phase, that is bounded by significantly lower critical fields than previously studied compounds (~0.4 T to 1.3 T) owing to weak superexchange interactions between 4f moments. The high-field part of the BEC-like dome is interrupted by an unusual regime indicated by unexpected signatures in the specific heat and ultrasound velocity data. Our results on Yb₂Si₂O7 provide the opportunity to study how anisotropic exchange and frustration in strongly spin orbit coupled materials modifes the field induced phases of the canonical quantum dimer magnet system.

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## Unidirectional Magnetization Dynamics in a Chiral Ice.

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Artificial spin ice [1] consists of geometrically frustrated arrangements of elongated nanomagnets. The magnetization in the single-domain nanomagnets points in one of two orientations along the magnet long axis as a result of the shape anisotropy. Tuning the dipolar interactions in such nanomagnet systems can lead to interesting collective behavior including emergent magnetic monopoles [2] and phase transitions [3]. In the work presented here, a collective clockwise rotation of the magnetization is demonstrated in a thermally-active system with a modified square-ice geometry [4], a so-called chiral ice where energy is converted into unidirectional dynamics. Using synchrotron x-ray photoemission electron microscopy, we observed how the collective rotation of the average magnetisation proceeds in a unique sense during thermal relaxation at room temperature. We clarified with micromagnetic simulations that this emergent chiral behavior is driven by the topology of the magnetic stray field at the edges of the nanomagnet array, resulting in an asymmetric energy landscape. Indeed, the stray field displays a complex topology characterized by the presence of antivortex patterns. The chiral ice can therefore effectively be seen as a virtual antivortex crystal, whose symmetry is broken at the edges, favoring the measured non-reciprocal dynamics. This thermally driven spin ice ratchet is interesting for novel nanoscale devices, such as magnetic nanomotors, actuators, sensors or memory cells.

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## Magnon triple points, topological transitions, and thermal Hall effect in pyrochlore iridates

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Triple points, triply degenerate band crossings, have been recently identified as a new type of fermion realized in electronic systems. We present a bosonic analog of a triple point topological semimetal. We theoretically show that such triple points can arise in the magnon band structure of pyrochlore iridates with the all-in-all-out antiferromagnetic order. By controlling the strength of Dzyaloshinskii-Moriya (DM) interaction in our spin model, we find three distinct regimes of magnon band topology, distinguished by different configurations of triple points in the Brillouin zone. We calculate the thermal Hall conductivity as an experimental probe of the magnon band topology. We find that the three regimes exhibit qualitatively different magnon thermal Hall effect. Particularly, in a regime relevant for real materials, the system shows a characteristic thermal Hall response that can be used to estimate the size of the DM interaction in experiments. (arXiv:1712.08170)

## Magnetic field dependences of magnetic susceptibilities and low energy excitations of frustrated spin system $RBaFe_4O_7$ (R=Ho, Tm)

- Using magnetic susceptibility and inelastic neutron scattering measurement -.

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RBaFe<sub>4</sub>O<sub>7</sub> (RBFO) (R = Ho and Tm) is considered as a 3-dimensional classical frustrated spin system. The antiferromagnetic RBFO has cubic symmetry, and Fe<sup>2+</sup> and Fe<sup>3+</sup> reside on corner-sharing-tetrahedra with a number ratio of 3: 1. Both R = Ho and Tm system do not show any static lattice distortion to the lowest temperature that we measured, even though Fe<sup>2+</sup> in tetrahedral symmetry is a Jahn-Teller active ion. The magnetic susceptibility of the R = Ho system is influenced by the strength of magnetic field, that is, the effective magnetic moment and the Curie -Weiss temperature depend on the strength of magnetic field. On the other hand, such behaviors of the R = Tm system is not affected by the strength of magnetic field. Although the former can be explained plausibly by existing of low energy excitation, observed energy levels which are obtained from the inelastic neutron scattering investigation of RBFO (R = Ho and Tm) powder samples are inconsistent with the energy scale of the strength of magnetic field and/or temperature in the magnetic susceptibility measurements. Magnetic field dependence of the magnetic susceptibility can be also confirmed even in another frustrated system, e.g. spinel and garnet, but whether the phenomena arise or not depend on a case-by-case. We would like to discuss whether the origin of the behavior comes from frustration effect or not.

#### Multiferroics by design: how to build multiferroic materials with frustrated molecular quantum magnets.

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Frustrated quantum magnetism has been the focus of intense research over many decades. Recently, it was realized that geometric frustration in Mott insulators can induce perturbative electron fluctuations controlled by spin configurations [1]. The simplest example is an equilateral triangle of spins with S=1/2, in which low-energy degrees of freedom consist of built-in magnetic and electric dipoles arising from the frustrated exchange interaction; such spin-trimers can be weakly coupled to make "multiferroics by design" [2]. Here we show that an organic molecular magnet known as TNN is an ideal building block for this novel mechanism of multiferroics, with the three spin-1/2 nitronyl nitroxide radicals in a perfect  $C_3$ -symmetric arrangement. As demonstrated by recent experiments (magnetization, ac dielectric constant, specific heat, and magnetic torque measurements) on a single crystal of TNN-CH<sub>3</sub>CN, the experimental thermodynamic phase diagram is in excellent agreement with our theory, which predicts multiferroic behavior and strong magnetoelectric effects arising from an intriguing interplay between magnetism and

effective orbital degrees of freedom [3]. Our study thus opens up new avenues for designing multiferroic materials using frustrated molecular magnets.

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## Random singlet and spin glass states in the S=1/2 triangular-lattice

Heisenberg model with random ferro- and antiferromagnetic interactions

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The "random singlet" (RS) state has been recently proposed as the ground state of the bond-random S=1/2 frustrated Heisenberg antiferromagnet [1-4]. The RS state is the resonating-valence-bond-like state where spin-singlet configurations are restricted due to quenched disorder. Meanwhile, it is still unclear whether the RS state is stable against gradual substitutions of ferromagnetic (FM) interactions for antiferromagnetic (AFM) ones. To clarify this matter, we study ground state properties of the bond-random S=1/2 triangular-lattice Heisenberg model with nearest-neighbor FM and AFM interactions by means of the exact diagonalization method. The model Hamiltonian is  $\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij} S_i \cdot S_j$ , where  $J_{ij}$  is the random nearest-neighbor interaction obeying the uniform distribution between  $[\bar{J} - \Delta, \bar{J} + \Delta]$  with  $\Delta = 1$ . The parameter  $\bar{J}$  measures the ratio of the FM bonds to AFM ones.  $\bar{J} = 1$  corresponds to the strongly-random AFM model in which the RS is reported to be stable [1,3]. With decreasing  $\bar{J}$ , the proportion of the FM bonds increases, and  $\bar{J} = 0$  corresponds to the so-called spin glass (SG) model with equal weight of the FM and AFM bonds. We computed the spin freezing parameter which can detect any magnetic order including the SG order. It is found that with decreasing  $\bar{J}$  (increasing FM bonds), the RS state becomes unstable and that a transition from the RS state to the SG state occurs at a critical value of  $\bar{J}_c \simeq 0.5$ . [1] K. Watanabe, et al., J. Phys. Soc. Jpn. 83, 034714 (2014); [2] H. Kawamura, et al., J. Phys. Soc. Jpn. 83, 103704 (2014); [3] T. Shimokawa, et al., Phys. Rev. B 92, 134407 (2015); [4] K. Uematsu and H. Kawamura, J. Phys. Soc. Jpn. 86, 044704 (2017).

#### Ground-state and Finite-temperature Properties of the Bilayer Kitaev model

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Recently, quantum spin liquid state in the two-dimensional Kitaev model [1] has attracted much interest since the Mott insulators with honeycomb-based structure have been synthesized such as  $A_2 \text{IrO}_3(A = \text{Na, Li})$  [2,3] and  $\alpha$ -RuCl<sub>3</sub> [4,5]. Most of theoretical studies focus on the two-dimensional Kitaev model, while the above Kitaev-candidates show the magnetic order at low temperatures. Therefore, it is necessary to discuss the effect of the interlayer coupling on the ground state and finite temperature properties. In this work, we consider the bilayer Kitaev model as a simple model to discuss the effect of the interlayer coupling. The model Hamiltonian is given as,

$$H = -J \sum_{\langle i,j\rangle_{\mu},\alpha} S^{\mu}_{i\alpha} S^{\mu}_{j\alpha} + J' \sum_{i} \mathbf{S}_{i1} \cdot \mathbf{S}_{i2}, \tag{1}$$

where  $S_{i,n}^{\alpha}$  is an s=1/2 spin operator at site i of the  $\alpha(=1,2)$ th layer, J is the Kitaev exchange and J' is the interlayer exchange. An important point is that the model has distinct singlet ground states in certain limits. When J'=0, the system is reduced to two independent Kitaev models, where a gapless quantum spin liquid is realized. On the other hand, when J=0, the ground state is a direct product of the dimer singlet with the gap. Therefore, a naive question arises whether or not the quantum phase transition between two disordered states occurs. To clarify this, we make use of the dimer expansion, bond operator and the exact diagonalization to determine the ground state phase diagram. Furthermore, we use the thermal pure quantum state [6] to clarify how the specific heat and entropy are affected by the interlayer coupling [7].

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#### Localized magnetic excitations of the strongly frustrated dimerized quantum magnet.

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A coupled spin dimer system has attracted considerable attention owing to a rich variety of intriguing quantum phenomena. Ba<sub>2</sub>CoSi<sub>2</sub>O<sub>6</sub>Cl<sub>2</sub> is magnetically described as a two-dimensional XXZ dimerized magnet with an effective spin S = 1/2 at low temperatures [1]. The ground state is a nonmagnetic singlet with a finite gap to the first excited triplet state. When magnetic field exceeding the gap energy is applied, magnetic excitations, magnons, are mapped onto the boson lattice. Previous high-field magnetization measurements have revealed that Ba<sub>2</sub>CoSi<sub>2</sub>O<sub>6</sub>Cl<sub>2</sub> exhibits a stepwise magnetization process with a plateau at one-half of the saturation magnetization, independently of field directions [1]. This suggests that the interdimer exchange interactions is fully frustrated in this compound and, hence, magnons form a periodic array regarded as a Wigner crystal in the plateau region. Here, we report magnetic excitations of Ba<sub>2</sub>CoSi<sub>2</sub>O<sub>6</sub>Cl<sub>2</sub> directly probed via inelastic neutron scattering measurements at 4 K. It is found that magnetic excitations observed at 4.8, 5.8, 6.6, and 11.3 meV are all resolution-limited and dispersionless, consistent with the previous magnetization studies. The excitation at 5.8 meV is assigned as singlet-triplet excitations to  $S^z = \pm 1$  states. Interestingly, neutron scattering intensities of three excitations at 4-7 meV exhibit different Q-dependences. In the presentation, we will discuss the origin of the observed excitations.

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## Beyond conventional magnetic order in the Shastry-Sutherland frustrated magnet TmB<sub>4</sub>

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Geometrically frustrated lattices such as the 2D Shasty-Sutherland lattice are known to induce emergent quantum phenomena such as spin liquids, topologically protected states, and complex magnetic order. The spin liquid  $SrCu_2(BO_3)_2$  is a famous example of the physical realisation of the Shasty-Sutherland lattice lattice in an insulator [1], yet there exists a family of rare-earth metal tetraborides that exhibit both lattice-induced geometrical frustration and itinerant behavior [2]. In this context, the magnetic order in the frustrated magnet  $TmB_4$  is of particular interest. The arrangement of the Tm rare-earth moments in each layer are indeed topologically equivalent to the 2D Shasty-Sutherland lattice while the crystal field effects lead to a strong Ising anisotropy. Unlike  $SrCu_2(BO_3)_2$ , antiferromagnetic order has been shown to exist in  $TmB_4$  below 10 K. Nevertheless, competing interactions lead to a complex magnetic-temperature phase diagram [3], with unusual evolution of the magnetic order. Additional interest in  $TmB_4$  is driven by the emergence of fractionalized magnetization plateaus as seen in  $SrCu_2(BO_3)_2$  [4].

Through measurements of neutron diffuse magnetic scattering and resonant soft X-ray scattering, we have demonstrated the co-existence of magnetic order with short-ranged correlations induced by the frustrated exchange interactions in TmB<sub>4</sub>. In addition, I will discuss the commensurate antiferromagnetic and three incommensurate magnetic phases with strong history-dependent interconversion hosted by the temperature-field magnetic phase diagram. Using a reproducible protocol for single crystal neutron scattering experiments in such a history-dependent system, we have established the evolution of the unconventional magnetic ordering in TmB<sub>4</sub> as a function of temperature and applied field.

## Strongly correlated metallic state in doped pyrochlore iridates Y<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> K. Matsuhira (Kyushu Inst. Tech.), T. Taniguchi (Kyushu Inst. Tech.), H. Nomura (Kyushu Inst. Tech.),R. Shibahara

(Kyushu Inst. Tech.), J. Angel (RIKEN), R. Asih (RIKEN), and I. Watanabe (RIKEN) —

Pyrochlore iridate Y<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> is known as Mott insulator and is theoretically predicted to exhibits AFM transition at 165 K with Ir moments with "all-in/all-out" configuration [1-3]. Theoretical study for pyrochlore iridates predict a new QCP around the disappearance of AFM with "all-in/all-out" configuration by chemical doping [4]. We have investigated the effect of chemical carrier doping for pyrochlore iridates in order to reveal the theoretically predicted QCP and new phase. In this presentation, we will show the effect of hole doping for Y<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> by substituting Y ions for both Ca ions and Cu ions. By the hole doping, the AFM ordering is rapidly suppressed. The doped sample of Cu5% and Ca20% shows metallic conductivity and has no LRO down to 0.35 K. Then, the resistivity shows T<sup>0.67</sup> dependence, suggesting QCP behavior. As the enhanced Wilson ratio is observed in the metallic state, a strongly correlated metallic state is realized.

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## Impact of Charge Disorder on Ln<sub>2</sub>ScNbO<sub>7</sub> Rare Earth Pyrochlores.

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The sensitivity of frustrated magnetism to small amounts of chemical disorder has been well documented and promoted studies on doping magnetic ions into the rare earth pyrochlores. This disorder or off-stoichiometry is capable of inducing new ground states among sensitive systems such as Tb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> and Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>. Other systems including the classical spin ice phases remain stable given small amounts of disorder. The rare earth pyrochlores Ln<sub>2</sub>Sc<sup>+3</sup>Nb<sup>+5</sup>O<sub>7</sub> provide an opportunity to investigate local charge induced disorder while keeping an ideal, stoichiometric magnetic lattice. Of the (+3,+5) systems, this series allows for convenient single crystal growth through the floating zone method encouraging the comparison of these systems to their conventional pyrochlore analogues by neutron scattering techniques. This disorder seems to be capable of anisotropically increasing antiferromagnetic exchange in the classical spin ice Dy<sub>2</sub>ScNbO<sub>7</sub> as well as suggesting that the monopole crystallization found in Nd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>[1] is a robust phase in the presence of local disorder.

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## Stability of the spiral spin liquid in MnSc<sub>2</sub>S<sub>4</sub>.

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We investigate the stability of the spiral spin-liquid phase in  $MnSc_2S_4$  against thermal and quantum fluctuations as well as against perturbing effects of longer-range interactions. Employing *ab initio* DFT calculations we propose a realistic Hamiltonian for  $MnSc_2S_4$ , featuring second  $(J_2)$  and third  $(J_3)$  neighbor Heisenberg interactions on the diamond lattice that are considerably larger than previously assumed. We argue that the combination of strong  $J_2$  and  $J_3$  couplings reproduces the correct magnetic Bragg peak position measured experimentally. Calculating the spin-structure factor within the pseudofermion functional-renormalization group technique we find that close to the magnetic phase transition the sizeable  $J_3$  couplings induce a strong spiral selection effect, in agreement with experiments. With increasing temperature the spiral selection becomes weaker such that around three times the ordering temperature an approximate spiral spin-liquid is realized in  $MnSc_2S_4$ .

## Spin-liquid-like state observed in a S=1/2 square-lattice antiferromagnet.

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The S=1/2 square-lattice Heisenberg model is one of the most studied models in frustrated magnetism. The frustration arises from the competition of two antiferromagnetic interactions: the nearest-neighbor  $J_1$  (side of the square) and the next-nearest neighbor  $J_2$  interaction (diagonal). A dominant  $J_1$  interaction ( $J_2/J_1 \ll 0.5$ ) results in Néel antiferromagnetic order whereas a dominant  $J_2$  ( $J_2/J_1 \gg 0.5$ ) results in columnar antiferromagnetic order. The ground state in the highly frustrated  $J_2/J_1 \approx 0.5$  region is under debate with many predictions of quantum spin liquid (QSL) or valence bond solid ground states. A number of experimental realizations of this model are known, but none are in the highly frustrated region.

Recently it was found that the isostructural  $\mathrm{Cu}^{2+}$  B-site ordered double-perovskites  $\mathrm{Sr}_2\mathrm{Cu}\mathrm{TeO}_6$  and  $\mathrm{Sr}_2\mathrm{Cu}\mathrm{WO}_6$  are S=1/2 Heisenberg square-lattice antiferromagnets with Néel  $(J_2/J_1=0.03,\,T_N=29\,\mathrm{K})$  and columnar order  $(J_2/J_1=7.92,\,T_N=24\,\mathrm{K})$ , respectively [1,2]. These compounds are on the opposite sides of the phase diagram with the highly frustrated region in-between. Here I report on the properties of the 1:1 solid solution  $\mathrm{Sr}_2\mathrm{Cu}(\mathrm{Te}_{0.5}\mathrm{W}_{0.5})\mathrm{O}_6$  [3]. This material has a spin-liquid-like ground state with many of the properties expected for a gapless QSL. The low-temperature magnetic specific heat is T-linear indicating gapless excitations. No magnetic order or static magnetism is observed with muon spin spectroscopy down to 19 mK. Moreover, the muon spin relaxation rate plateaus below 0.5 K. The possibility of a QSL-like disorder-induced random-singlet state is also discussed [4].

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## Waiting time effects on the density of monopoles in spin ice Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>

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In spin ice materials below 200mK the dynamics are dominated by monopoles. By thermally quenching spin ice to millikelvin temperatures using the avalanche quench protocol[1], we can prepare a large, far from equilibrium density of metastable magnetic monopoles. We use this approach to study the spin ice material  $Ho_2Ti_2O_7$  and have measured the monopole [2] current as well as the field at which avalanches occur while ramping up the field. Emphasis was put on the waiting time after the quench and before the measurements begin, showing rapid recombination of monopoles even at 200 mK. Comparison of the results with  $Dy_2Ti_2O_7$  gives insights to the tunneling mechanism governing the hopping of monopoles on the lattice. The non-standard techniques used to make these measurements will be presented, as well as new results.

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#### Probing emergent excitations in $Pr_2Hf_2O_7$ with thermal conductivity

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Pr<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub> (PHO) is a quantum spin ice candidate with a non-Kramers doublet ground state that displays evidence of dynamic spin ice behaviour [1][2]. We report thermal conductivity measurements of single crystal samples of PHO as a function of temperature between 50 mK and 1 K and magnetic field up to 12 T. The high field measurements are to identify the lattice contribution through polarizing the magnetic spins. However, the application of a magnetic field up to 14 T does not appear to saturate its magnetization at 2 K [1]. To understand phonon transport in PHO, we report thermal conductivity measurements of different sized samples. We interpret our results considering current theoretical predictions for exotic excitations in quantum spin liquids, such as emergent photons, magnetic monopoles and visons [3].

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## Short range order in the quantum XXZ honeycomb lattice material BaCo<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>

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We present observations of highly frustrated quasi two-dimensional (2D) magnetic correlations in the honeycomb lattice layers of the  $S_{eff}$ = 1/2 compound  $\gamma$ -BaCo<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub> ( $\gamma$ -BCPO). Specific heat shows a broad peak comprised of two weak kink features at  $T_{N1} \sim 6$  K and  $T_{N2} \sim 3.5$  K, the relative weights of which can be modified by sample annealing. Neutron powder diffraction measurements reveal short range quasi-2D order that is established below  $T_{N1}$  and  $T_{N2}$ , at which two separate, incompatible, short range magnetic orders onset: commensurate antiferromagnetic correlations ( $T_{N1}$ ) and in quasi-2D helical domains ( $T_{N2}$ ). The ac magnetic susceptibility response lacks frequency dependence, ruling out spin freezing. Inelastic neutron scattering data on  $\gamma$ -BCPO is compared with linear spin wave theory, and two separate parameter regions of the XXZ  $J_1$ - $J_2$ - $J_3$  model with ferromagnetic nearest-neighbor exchange  $J_1$  are favored, both near regions of high classical degeneracy. High energy coherent excitations ( $\sim 10$  meV) persist up to at least 40 K, suggesting strong in-plane correlations persist above  $T_N$ . These data show that  $\gamma$ -BCPO is a rare highly frustrated, quasi-2D  $S_{eff}$  = 1/2 honeycomb lattice material which resists long range magnetic order and spin freezing.

H.S. Nair, J.M. Brown, E. Coldren, G. Hester, M.P. Gelfand, A. Podlesnyak, Q. Huang, K.A. Ross. arXiv:1712.06208 [cond-mat.str-el] (2017)

# Successive magnetic phase transitions and magnetization plateau in the spin-1 triangular-lattice antiferroagnet $Ba_2La_2NiTe_2O_{12}$

M. Saito (Tokyo Institute of Tech.), M. Watanabe (Tokyo Institute of Tech.), N. Kurita (Tokyo Institute of Tech.), H. Tanaka (Tokyo Institute of Tech.), A. Matsuo (ISSP, Univ. Tokyo), and K. Kindo (ISSP, Univ. Tokyo) — Triangular-lattice antiferromagnets (TLAFs) have been studied vigorously because of the remarkable quantum many-body effects, which originate from the geometric frustration and quantum fluctuation. On the experimental side, search of model substances and measurements of their physical properties have been performed actively. Recently the magnetic properties of  $A_4MB_2O_{12}$  type compounds (A = Ba, Sr, La; M = Co, Ni, Mn; B = W, Re), in which magnetic  $M^{2+}$  ions form uniform triangular lattice, have been reported. However, the exchange interactions were found to be ferromagnetic except for  $Ba_2La_2NiTe_2O_{12}$  with spin-5/2 [1,2].

In this study, we synthesized  $Ba_2La_2NiTe_2O_{12}$  and investigated its magnetic properties. Although the crystal structure of this compound is the same as that of  $Ba_2La_2NiW_2O_{12}$ , the exchange interaction is expected to be antiferromagnetic and large from the viewpoint of exchange path  $Ni^{2+}-O^{2-}-Te^{6+}-O^{2-}-Ni^{2+}$  [3,4]. Magnetic susceptibility and heat capacity measurements revealed that the exchange interaction is antiferromagnetic and large, i.e.,  $J/k_B \sim 20$  K, and that successive magnetic phase transitions occur at  $T_{N1}=9.8$  K and  $T_{N2}=8.9$  K. Weak ferromagnetic moment was also observed in the ordered states. It was found from high-magnetic-field magnetization measurement, that the magnetization curve exhibits a plateau at one-third of the saturation magnetization, which is characteristic of triangular-lattice quantum antiferromagnet. Although the exchange interaction in  $Ba_2La_2NiW_2O_{12}$  is similar to that in  $Ba_3NiSb_2O_9$  [5], the field range of the magnetization plateau in  $Ba_2La_2NiW_2O_{12}$  is more than twice that in  $Ba_3NiSb_2O_9$  [5]. These experimental results indicates that the magnetic anisotropy is easy-axis type and the interlayer exchange interaction is ferromagnetic in contrast with the antiferromagnetic interlayer exchange interaction in  $Ba_3NiSb_2O_9$ .

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## High-pressure phases of Kitaev materials (as seen by muSR).

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Bond-dependent interactions between magnetic moments can lead to strong frustration and nontrivial ground states. In particular, the Kitaev-Heisenberg model has a rich phase diagram and can host a spin liquid state or different frozen states depending on the strength of the additional Heisenberg interactions. Experimentally such phase diagrams can be explored by modifying the relative interaction strengths in materials by applying pressure.

In this presentation I will describe how the muon spin rotation technique can be used to study such materials under applied pressure and what it can reveal about the transitions between different phases. I will then show examples of our recent high-pressure studies in Kitaev candidate materials based on iridium, including the suppression of magnetic ordering in  $\beta$ -Li<sub>2</sub>IrO<sub>3</sub>. Finally, I will discuss the high-pressure phase in  $\alpha$ -RuCl<sub>3</sub> and possible scenarios that can be responsible for it.

## Numerical analysis for Berezinskii-Kosterlitz-Thouless transitions with incommensurate orders.

M. Tabata, D. Yamamoto and N. Furukawa (Dept. Phys, Aoyama Gakuin Univ.) —

We study magnetic phase diagrams of classical Heisenberg models on a spatially anisotropic triangular lattice. Such models are canonical systems to study order-by-disorder phenomena where degeneracies of classical ground states are lifted by thermal (or quantum, in other cases) fluctuations. In the extensively studied case where spin exchange couplings are spacially isotropic [1,2], where the degenerate ground-state manifold contains commensurate collinear and coplanar ordered states, the order-by-disorder phenomena exhibit exotic magnetic states and non-trivial phase transition phenomena. In the presence of spacial anisotropies, the models prefers to show non-coplanar incommensurate ("cone") orders [3], which have prevented researchers to investigate the full magnetic phase diagram in detail with precisions. In the present study, we have developed a novel Monte Carlo analysis using optimized boundary conditions [4], which enabled us to study systematic finite size scalings in the BKT transitions of incommensurate magnetic orders with precisions. This method is also applicable to other incommensurate systems which exhibit BKT transitions.

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## Ground-state and Finite-temperature Properties of the Bilayer Kitaev model

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Recently, quantum spin liquid state in the two-dimensional Kitaev model [1] has attracted much interest since the Mott insulators with honeycomb-based structure have been synthesized such as  $A_2 \text{IrO}_3(A = \text{Na}, \text{Li})$  [2,3] and  $\alpha$ -RuCl<sub>3</sub> [4,5]. Most of theoretical studies focus on the two-dimensional Kitaev model, while the above Kitaev-candidates show the magnetic order at low temperatures. Therefore, it is necessary to discuss the effect of the interlayer coupling on the ground state and finite temperature properties. In this work, we consider the bilayer Kitaev model as a simple model to discuss the effect of the interlayer coupling. The model Hamiltonian is given as,

$$H = -J \sum_{\langle i,j\rangle_{\mu},\alpha} S^{\mu}_{i\alpha} S^{\mu}_{j\alpha} + J' \sum_{i} \mathbf{S}_{i1} \cdot \mathbf{S}_{i2}, \tag{2}$$

where  $S_{i,n}^{\alpha}$  is an s=1/2 spin operator at site i of the  $\alpha(=1,2)$ th layer, J is the Kitaev exchange and J' is the interlayer exchange. An important point is that the model has distinct singlet ground states in certain limits. When J'=0, the system is reduced to two independent Kitaev models, where a gapless quantum spin liquid is realized. On the other hand, when J=0, the ground state is a direct product of the dimer singlet with the gap. Therefore, a naive question arises

whether or not the quantum phase transition between two disordered states occurs. To clarify this, we make use of the dimer expansion, bond operator and the exact diagonalization to determine the ground state phase diagram. Furthermore, we use the thermal pure quantum state [6] to clarify how the specific heat and entropy are affected by the interlayer coupling [7].

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## Investigations of scaling and dynamics in the kagomé ice phase of Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>

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Frustration of the exchange and dipolar interactions between Ising-like rare earth magnetic moments oriented along the pyrochlore easy axes produces a quasi-degenerate manifold of 2-in/2-out (ice rule) ground states in the spin ices Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> and Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> [1]. Applying a medium strength field along the [111] direction of a spin ice results in a magnetization plateau known as kagomé ice [2], where the pyrochlore lattice can be separated into stacked triangular and kagomé planes, with spins in the triangular planes being parallel to the field, while those in the kagomé planes are not. In kagomé ice, the ice rules compete with the applied field, favoring 2 in/1 out orientations on each triangle of the kagomé lattice, reducing both the degeneracy and the entropy of the system [3]. Kagomé ice is a two dimensional analog of spin ice with its own distinct set of spin correlations [4,5].

Kagomé ice hosts a variety of interesting phase transitions and crossovers with varying field and temperature, including a Kasteleyn transition as the field direction is tilted from the [111] towards the [112], the scaling for which can be observed in the structure factor of neutron scattering measurements [4–8]. The concentration of spin flip excitations in spin ice (recontextualized as magnetic monopole quasiparticles [9]) experiences various crossovers with increased field and temperature, including Kibble-Zurek scaling below the critical point [10] and peaks in the magnetization, specific heat [3] and susceptibility [11]. As the energy of spin flip excitations in the kagomé plane changes with the applied field, the mobility of monopole quasiparticles is constrained further from their spin ice counterparts. Using diffuse neutron scattering and high frequency susceptibility measurements on a single crystal sample of Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>, alongside Monte Carlo simulations, we have observed and characterized signals of the scaling near the Kasteleyn transition and crossovers attributed to changing monopole density above the critical point.

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## Inorganic and Inorganic-Organic Hybrid Analogues of $S = \frac{1}{2}$ Kagome Antiferromagnets.

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Frustrated  $S = \frac{1}{2}$  antiferromagnets combine geometrical frustration with quantum fluctuations, making these materials the perfect candidates for the elusive quantum spin liquid. Understanding the quantum states of matter in these materials may have important implications for revolutionary quantum technology, for example in quantum computers and sensors.

This work will focus on the development of new syntheses for experimental realisations of the quantum spin liquid in frustrated kagome antiferromagnets.

Much of the emphasis to date has been on materials in which Cu<sup>2+</sup> ions form layers of frustrated kagome lattices. One example which has drawn much attention is herbertsmithite, ZnCu3(OH)6Cl2 [1]. However, antisite Zn<sup>2+</sup>/Cu<sup>2+</sup> disorder and debate over the exact nature of the ground state in herbertsmithite calls for the synthesis of new candidate materials. Barlowite, Cu4(OH)6FBr, for example, orders magnetically at 15 K, but it has been suggested that doping the material with isoelectronic ions such as Zn<sup>2+</sup> and Mg<sup>2+</sup> may tune the structure to that of herbertsmithite [2]. Recent studies have shown that doping in as little as 40% of the interlayer site results in suppression of magnetic order [3]. Another class of promising materials are metal-organic frameworks (MOFs). One example is [Cu3(CO3)2(bpe)3]. 2ClO4 (bpe = 1,2-bis(4-pyridyl)ethane), in which antiferromagnetic interactions within the kagome layers and ferromagnetic coupling between these layers coexist [4]. It is hoped that these inorganic-organic hybrids offer the benefit of greater control over interlayer coupling through alteration of the organic component, as well as the possibility of adding further functionality. Current research efforts are focussed on developing the synthesis for doped barlowite, as well as iodide and chloride barlowite analogues. Magnetic susceptibility and muon spectroscopy measurements will be presented for samples containing varying levels of Zn<sup>2+</sup>. In addition, a library of layered MOFs has been synthesised based on a Solvay process previously reported [4]. The variation of the structural and magnetic properties in these systems will be demonstrated using powder and single crystal X-ray diffraction, in combination with magnetic susceptibility measurements. [1] M. P. Shores et al., J. Am. Chem. Soc. 127, 13462 (2005); [2] D. Guterding et al., Phys. Rev. B 12, 125136 (2016); [3] Z. Feng et al., arXiv.1712.06732v1 (2017); [4] P. Kanoo et al., Dalton Trans. 26, 5062 (2009).

## Magnetic clustering from Coulomb phase: fractionalization and recombination

M. Udagawa (Gakushuin Univ.), T. Mizoguchi (Gakushuin Univ.) and L. D. C. Jaubert (CNRS, Univ. Bordeaux)
Recently, fractionalization of elementary excitations is drawing considerable attention in frustrated magnets.
Fractionalization is a phenomenon where a natural quantum number of the system, such as charge and spin is fragmented into several components, and takes a smaller value than its basic unit. In this regard, "recombination" gives an interesting viewpoint: By recombining fractionalized excitations in a nontrivial way, it is possible to obtain a new phase or collective excitation that are hard to construct from the original spin or fermionic degrees of freedom.
In this contribution, we pursue this scenario, by taking up J<sub>1</sub>-J<sub>2</sub>-J<sub>3</sub> Ising model defined on pyrochlore and kagome lattices. The nearest-neighbor J<sub>1</sub> leads to the formation of spin-ice-type degenerate ground states, which support fractional monopole excitations. The monopoles have magnetic charges, which determine their creation-annihilation rule, i.e., positive monopoles pair-annihilate only with negative charges. The farther-neighbor J<sub>2</sub> and J<sub>3</sub>, introduce short-range interactions between monopoles. Positive (Negative) J leads to attractive (repulsive) interaction between like charges.

In particular, in the case of positive *J*, the monopole excitations exhibit non-trivial recombination. In this case, like charges tend to form a cluster, however, they are prohibited to pair-annihilate due to the constraint of local charge conservation. As remarkable consequences of these interplay, we will report the formation of novel classical spin liquid in the kagome model [1], and a novel collective excitation stabilized in the pyrochlore system [2], and discuss their physical consequences for experimental observables. We further extend our analysis to the case of continuous spins [3], and address the clustering of magnetic excitations.

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## Exact Diagonalization of a Quantum XXZ Model with Long-Range Interactions.

Christopher N. Varney(UWF), Spencer Leeper(UWF), Roger Johnson (UWF) and David Smith (UWF,VTech) — Advancements in utilizing ultra-cold gases as quantum spin simulators are allowing for the exploring the exotic states and excitations of spin-1/2 systems on frustrated lattices. Long-range interactions can also frustrate the spins and competition between the geometric frustration and long-range interactions makes the underlying orders in the ground

state unclear. Here we investigate the ground state phase diagram of the quantum dipolar XXZ model on a square lattice with exact diagonalization to characterize the effects of the long-range interactions.

## Evolution of spin correlations in SrDy<sub>2</sub>O<sub>4</sub> in zero and applied magnetic fields

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Frustrated magnetism is the study of competing interactions, and when these are incompatible with the geometry of the lattice, systems often show non-trivial behaviour and can even find it hard to establish a unique ground state. Using bulk property measurements, neutron diffraction and simulations we report on the development of short- and long-range magnetic order induced in a frustrated 1D spin-chain compound  $SrDy_2O_4$  in zero and applied magnetic fields. In  $SrDy_2O_4$  there are two magnetic sites, and strong crystal field and single-ion anisotropies combine to allow the Dy ions to behave as Ising spins which point along orthogonal crystallographic axes. In zero field there is no long-range order down to 60 mK, but diffuse scattering reflects that the spin arrangements remain correlated but fluctuating - a complex middle ground between liquid-like randomness and periodic order. In-field measurements further reflect the unusual and highly anisotropic nature of  $SrDy_2O_4$ .

O.A. Petrenko et al., Phys. Rev B 95 104442 (2017)

## Generalized XY model with antiferronematic interaction

M. Žukovič (Institute of Physics, P.J. Šafárik University, Slovakia)

A generalized ferromagnetic (FM) XY model that includes a nematic term has been intensively studied in connection with various experimental realizations, such as liquid crystals [1,3], superfluid A phase of <sup>3</sup>He [2], or high-temperature cuprate superconductors [4]. From a theoretical point of view such a model shows an interesting critical behavior with separate magnetic and nematic quasi-long-range order (QLRO) phases and the respective phase transitions belonging to different universality classes [1,2]. In the case of the geometrically frustrated model on a triangular lattice with antiferromagnetic (AFM) and antiferronematic (AFN) interactions another chiral long-range order phase, which can also exist in the absence of magnetic order, has been confirmed [5]. Geometrically frustrated models with the magnetic and nematic couplings having opposite signs have been proposed in the interdisciplinary applications for modeling of DNA packing [6] and structural phases of cyanide polymers [7,8].

In the present investigation we consider the XY model with the FM and AFN nearest-neighbor interactions on a square lattice for a varying interaction strength ratio. Besides the FM and AFN QLRO phases we identify at low temperatures another peculiar canted ferromagnetic (CFM) QLRO phase, resulting from the competition between the collinear FM and non-collinear AFN ordering tendencies. In the CFM phase neighboring spins that belong to different sublattices are canted by a non-universal (dependent on the interaction strength ratio) angle and the ordering is characterized by a fast-decaying power-law intra-sublattice correlation function. Compared to the FM QLRO phase, in the CFM QLRO phase the correlations are significantly diminished by the presence of zero-energy domain walls due to the inherent degeneracy caused by the competing interactions. We present the phase diagram as a function of the interaction strength ratio and discuss the character of the respective phases as well as the transitions between them.

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## Possible gapless spin liquid in a rare-earth kagomé lattice magnet Tm<sub>3</sub>Sb<sub>3</sub>Zn<sub>2</sub>O<sub>14</sub>.

L. Shu, Z. F. Ding, Y. X. Yang, J. Zhang, C. Tan, Z. H. Zhu, and G. Chen (Fudan University)

We report the thermodynamic and muon spin relaxation ( $\mu$ SR) evidences for a possible gapless spin liquid in the recently discovered  $Tm_3Sb_3Zn_2O_{14}$ , with the rare-earth ions  $Tm^{3+}$  forming a two-dimensional kagomé lattice. We extract the magnetic specific heat of  $Tm_3Sb_3Zn_2O_{14}$  by subtracting the phonon contribution of the non-magnetic isostructural material  $La_3Sb_3Zn_2O_{14}$ . We obtain a clear linear-T temperature dependence of magnetic specific heat at low temperatures, with the heat-capacity coefficient  $\gamma=0.0266(1)$  J mol- $Tm^{-1}$  K $^{-2}$  in the zero temperature limit. No long-range magnetic order was observed down to 0.3 K in the heat capacity measurement. A broad hump around 6.5 K was observed in the zero field magnetic specific heat and is gradually suppressed in the magnetic fields that also creat a spin gap in the specific heat. The absence of magnetic order is further confirmed by the  $\mu$ SR measurement down to 20 mK. We find that the spin-lattice relaxation time remains constant down to the lowest temperatures. We point out that the physics in  $Tm_3Sb_3Zn_2O_{14}$  is fundamentally different from the Cu-based herbertsmithite and propose spin liquid ground states with non-Kramers doublets on the kagomé lattice to account for the experimental results.

## 0.22 Poster Session II

Wednesday 7/11

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1. C. Balz (ORNL)
               2. S. Chillal (Helmholtz-Zentrum Berlin)
                        3. S. Dey (TU Dresden)
               4. S. E. Dutton (University of Cambridge)
                   5. Shunsuke C. Furuya (RIKEN)
                         6. P Henelius (KTH)
                 7. K. Matsuhira (Kyushu Inst. Tech.)
                 8. H. O. Jeschke, Okayama University
               9. W. Jin (University of Waterloo, Canada)
            10. Wen-Han Kao (National Taiwan University)
                  11. Y. Kojima(Tokyo Inst. of Tech.)
                        12. J. Lass (Univ. Cph.)
                          13. C. Lee (OIST)
                       14. F.-Y. Li (Fudan Univ.)
                          15. C. Liu (UCSB)
                        16. C. Liu(Fudan Univ.)
          17. Michael J. Lawler (Cornell U., Binghamton U.)
          18. P. Mendels (Univ. Paris-Sud, Univ. Paris-Saclay)
                19. D. Maiti (SNBNCBS,kolkata,India)
                        20. P. Maksimov (UCI)
              21. Takahiro Misawa (ISSP, Univ. of Tokyo)
                        22. A. Mishra (KAIST)
                      23. Soshi Mizutani(OIST)
             24. W. M. H. Natori (University of Sao Paulo)
               25. K. Nawa (IMRAM Tohoku University)
      26. N. Swain (Nanyang Technological University, Singapore)
               27. J. Oitmaa (UNSW, Sydney, Australia)
               28. J. Oitmaa (UNSW, Sydney, Australia)
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                         30. J. C. Orain (PSI)
31. A. M. Oleś (M. Smoluchowski Institute Poland, Max Planck Stuttgart)
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        34. J. Paddison (University of Cambridge/Georgia Tech)
                     35. C. Pasco (Johns Hopkins)
                    36. N. Perkins (U. Minnesota)
                     37. W. E. Pickett (UC Davis)
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                         39. X. Plat (RIKEN)
                 40. Krishanu Roychowdhury (Cornell)
                  41. Megan Rutherford (UWinnipeg)
                   42. K. Tomiyasu (Tohoku Univ.)
                       43. Zhentao Wang (UTK)
             44. M. Watanabe(Tokyo Inst. of Tech., Japan)
                       45. M. G. Yamada (ISSP)
                         46. Han Yan (OIST)
                 47. M. Ye (University of Minnesota)
                 48. A. Yaresko (MPI FKF, Stuttgart)
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## Polarized neutron study of $\alpha$ -RuCl<sub>3</sub>.

C. Balz (ORNL), A. Banerjee (ORNL), P. Lampen-Kelley (UTK), D. G. Mandrus (UTK), and S. E. Nagler (ORNL)

The magnetic insulator  $\alpha$ -RuCl<sub>3</sub> features a layered honeycomb structure of edge-sharing octahedrally coordinated Ru<sup>3+</sup> ions satisfying the conditions necessary for producing Kitaev couplings. Though it orders magnetically at low temperatures in zero-field, it exhibits a continuum of magnetic excitations previously identified as a signature of fractionalized excitations characteristic of quantum spin liquids.

Here we report our recent polarized neutron scattering measurements enabled through the availability of large high-quality single crystals. Polarized elastic scattering allows for a direct determination of the direction of the ordered spin moment while inelastic scattering confirms the magnetic nature of the excitations seen above and below  $T_N$ . Polarized inelastic scattering further provides information about the direction in which the spins fluctuate. The data enables us to distinguish between the transverse and longitudinal excitation components of the magnetic response revealing intricate details of the fluctuation mechanisms important for further theoretical understanding.

#### A quantum spin liquid based on a new three dimensional lattice.

S. Chillal (Helmholtz-Zentrum Berlin), Y. Iqbal (IIT Madras), H. O. Jeschke (Okayama University), J. A. Rodriguez-Rivera (NIST, University of Maryland), R. Bewley (ISIS Facility), P. Manuel (ISIS Facility), D. Khalyavin (ISIS Facility), P. Steffens (Institut Laue-Langevin), R. Thomale (Julius-Maximilian's University of Würzburg), A. T. M. N. Islam (Helmholtz-Zentrum Berlin), J. Reuther (Helmholtz-Zentrum Berlin, Freie Universität Berlin), and B. Lake (Helmholtz-Zentrum Berlin, Technische Universität Berlin)

Quantum spin liquid (QSL) is a highly entangled magnetic state found in frustrated magnetic systems. This is generally characterized by the absence of static magnetism together with the presence of highly correlated excitations known as spinons. In systems with isotropic interactions, such phenomenon is usually sought in lattices where magnetic ions form triangular or tetrahedral arrangements and are interacting via antiferromagnetic interactions. Several compounds have been reported to show the spin liquid behaviour in two dimensionally frustrated lattices such as the kagome in Herbertsmithite and Kitaev Honeycomb in alpha-RuCl<sub>3</sub>. In three dimensions, the experimental realization is mostly limited to pyrochlore systems which are formed by corner-shared tetrahedra. Whereas, three-dimensional networks of corner-sharing triangles such as hyperkagome lattice are very rare. In this context, we explore a new three-dimensional magnet PbCuTe<sub>2</sub>O<sub>6</sub>, consisting of antiferromagnetically coupled S- $\frac{1}{2}$  ions that form a three-dimensional network of corner-sharing triangles. This lattice, which we define as the hyper-hyperkagome, has three triangles connected per magnetic ion and hence is distinctly different from the generally known hyperkagome. By performing a combined dc susceptibility and neutron scattering experiments we confirm that its ground state does not develop any static magnetism and its excitations form diffuse, dispersionless spheres suggesting spinon excitations. Together, these results point to a quantum spin liquid state in the new three dimensionally frustrated hyper-hyperkagome lattice. Furthermore, with the help of Curie-Weiss temperature from dc susceptibility and density functional theory calculations we determine the magnetic Hamiltonian which reproduces all crucial characteristics of the spin liquid behavior in PbCuTe<sub>2</sub>O<sub>6</sub>.

## Quenched bond disorder in a non-collinear antiferromagnet

S. Dey (TU Dresden) and M. Vojta (TU Dresden)

In antiferromagnets, the presence of geometric frustration often leads to classical ground states with non-collinear spin ordering. Quenched disorder is an interesting ingredient which tends to counteract spontaneous symmetry breaking in low dimensional systems. Consequently, the study of the interplay between disorder and frustration has garnered some serious attention recently [1,2]. To understand the resulting phenomena, we explore a generic point of view and in addition also focus on a prototypical example, the disordered triangular lattice antiferromagnet (TLAF) with next and next to nearest neighbor Heisenberg interaction. The homogeneous limit of this model hosts a phase transition between non-collinear antiferromagnetic LRO and what is believed to be a Z2 spin liquid [3]. Combining analytical arguments

and finite-system numerical simulations, we study the destruction of the LRO by bond disorder and discuss physical properties of the emergent state at low temperatures. We also connect our findings to recent experimental observations on related compounds, YbZnGaO<sub>4</sub> and YbMgGaO<sub>4</sub> [1].

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## Interplay of chemical pressure, spin isotropy and magnetic frustration in lanthanide garnets

S. E. Dutton (University of Cambridge), P. Mukherjee (University of Cambridge) and J. Paddison (University of Cambridge)

Lanthanide garnets  $Ln_3A_2X_3O_{12}$  have a highly frustrated magnetic  $Ln_{3+}$  lattice, in which the magnetic  $Ln_{3+}$  ions lie at the vertices of cornersharing triangles which form two interpenetrating networks of bifurcated ten-membered rings. Much of the experimental and theoretical work has focused on the spin liquid candidate gadolinium gallium garnet (GGG),  $Gd_3Ga_5O_{12}$ , however far less attention has been paid to the isostructural lanthanide gallium garnets,  $Ln_3Ga_5O_{12}$  Ln=Tb ,Dy, Ho, which exhibit substantial single ion anisotropy. In this presentation the role of chemical pressure by substitution on the A and X sites will be discussed. Specifically the changes in the magnetic properties on aliovalent doping[1] and relief of the magnetic frustration on magnetic substitution will be presented [2,3].

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## Theory of electron spin resonance for detecting long-range spin nematic orders.

Shunsuke C. Furuya (RIKEN) and Tsutomu Momoi (CEMS, RIKEN)

Spin nematic order is an interesting but "hidden" magnetic order characterized by a quadrupoler order parameter. Since it is coupled to neither the magnetic field nor the neutron, it is currently an important issue in the field of frustrated magnetism to develop a method for such a hidden magnetic order. In this presentation, we discuss that the electron spin resonance is effective for that purpose especially under the high magnetic field. First, we present a generic relation between the quadrupoler order parameter and the electron spin resonance in the presence of weak anisotropic interactions. Next, we show that a simple application of our generic theory to a specific two-dimensional quantum magnetic system and discuss implications of this theory to experiments. This presentation is based on our paper [1].

[1] Shunsuke C. Furuya and Tsutomu Momoi, arXiv:1707.08784.

## **Interaction Induced Special Temperatures in Frustrated Ferromagnets.**

P Henelius (KTH), L. Bovo (UCL), M. Twengström (KTH), O Petrenko (U. of Warwick), T. Fennell (PSI), M Gingras (U. of Waterloo) and S Bramwell (UCL)

The magnetic bulk susceptibility can be used to classify magnets as ferromagnets ( $\chi T/C > 1$ ) or antiferromagnets ( $\chi T/C < 1$ ). In this study we identify a new class of "inverting" magnets that exhibit a maximum in  $\chi T/C$  as a function of temperature. In analogy with classical gases we identify the peak temperature with a magnetic Joule temperature, where the system is quasi-ideal, dU/dM=0, and the onset of antiferromagnetic correlations. In addition, we find a magnetic Boyle temperature, where  $\chi T/C=1$ , and the incipient ferromagnet turns to an antiferromagnet at low temperature. We provide a phenomenological model of the susceptibility which reveals the mechanism that induces the special temperatures and elevates the effects of minute frustrated exchange interactions to surprisingly high temperature. By explicitly decomposing the dipolar Hamiltonian we demonstrate that these special temperatures and eventual antiferromagnetic ordering are caused by the quadrupolar corrections to a monopolar (dumbbell) Hamiltonian. Our study establishes  $\chi T/C$  as a direct measure of interaction parameters which are otherwise difficult to access experimentally. Since the special temperatures are indicative of the very low-temperature phases of the magnetic system, but occur at a higher and often more readily experimentally accessible temperature, we believe that they will be a useful diagnostic tool in the ongoing search for spin liquids. We find that a number of inverting magnets, including the spin ice materials Dy/Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>, kapellasite and the spinel GeCo<sub>2</sub>O<sub>4</sub> belong to this group.

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## Nonlinear conductivity of frustrated iridate Ca<sub>5</sub>Ir<sub>3</sub>O<sub>12</sub>

K. Matsuhira (Kyushu Inst. Tech.), K. Nakamura (Kyushu Inst. Tech.), Y. Yasukuni (Kyushu Inst. Tech.), Y. Yoshimoto (Univ. Tokyo), D. Hirai (ISSP, Univ. Tokyo) and Z. Hiroi (ISSP, Univ. Tokyo) —

We report the transport properties along the c-axis in a single crystal of  $Ca_5Ir_3O_{12}$  with narrow band gap [1]. In the crystal structure, it should be noted that 1D chains of the edge-sharing  $IrO_6$  form triangular lattices [2]. We discovered nonlinear conductivity in I-V relationship in the non-ordered state. The nonlinearity becomes stronger as temperature decreases. We also showed the *ab initio* density functional band structures and the Fermi surface. The estimated SOI is  $\sim 0.3$  eV, which is large enough to be comparable to the valence bandwidth of  $\sim 0.5$  eV. The SOI splits the metallic bands and leads to a pocket-like band structure, thus reducing the metallic trend. The Fermi surface has a sheet structure along the  $c^*$ -axis, due to the 1D chain structure of the edge-sharing  $IrO_6$ .

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## Identifying and predicting spin liquids materials using energy mapping methods.

H. O. Jeschke, Okayama University

We review the use of all electron density functional theory calculations to extract magnetic exchange couplings. By mapping the total energies of large numbers of different spin configurations to the Heisenberg Hamiltonian, we can achieve very precise information about the model describing a material. We show that this method often leads to very good agreement with experimental data. As examples, we discuss kagome, pyrochlore and diamond lattice materials. The mineral barlowite  $Cu_4(OH)_6FBr$  has recently been synthesized and characterized magnetically. Due to interstitial  $Cu^{2+}$  between perfect kagome layers it orders magnetically [1]. Theoretically, the hypothetical material  $ZnCu_3(OH)_6FBr$  has been postulated [2]. The exchange Hamiltonian obtained using energy mapping was found to be an antiferromagnetic kagome lattice with only a 6% subleading interlayer coupling. This makes the material a new candidate spin-liquid material which has recently been confirmed experimentally (Z. Feng et al., Chin. Phys. Lett. 34, 077502 (2017)). The recently synthesized oxynitride  $Lu_2Mo_2O_5N_2$  is a rare realization of an S=1/2 pyrochlore antiferromagnet. Energy mapping shows that it is likely to be in a spin-liquid region of the pyrochlore lattice because of rather than in spite of significant subleading exchange couplings [3].

The research was performed in collaboration with R. Valentí, F. Salvat-Pujol, D. Guterding, Y. Iqbal, T. Müller, J. Reuther, S. Rachel, R. Thomale and M. J. P. Gingras.

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#### Spin-current order in antiferromagnetic zigzag ladder.

W. Jin (University of Waterloo, Canada) and O. Starykh (University of Utah, USA)

Here we study the stability of the collinear up-up-down phase in the 1/3 magnetization plateau in a zigzag ladder, which is a frustrated spin chain with competing nearest and next-nearest neighbor coupling  $J_1$  and  $J_2$ . The classically unfavorable 1/3 magnetization plateau survives through a large range away from the Majumdar-Ghosh point  $(J_2/J_1=1/2)$ . Via the semi-classical large-S expansion, we find that near the end of plateau, quantum fluctuations induce a two-magnon instability. This instability corresponds to a spin current (bond nematic) state as was proposed in Phys. Rev. Lett. 110, 217210 (2013) for a two-dimensional spatially anisotropic triangular lattice antiferromagnet. We find that the width of this bond nematic phase scales  $1/\sqrt{S}$ , which is much stronger than  $1/S^2$  dependence found on the triangular lattice.

We propose  $CaV_2O_4$  [1] and  $Cu_3V_2O_7(OH)_2\cdot 2H_2O$  [2] as possible candidates to search for the experimental realization of spin nematic order in antiferromagnets. Unlike the ferromagnetic LiCuVO<sub>4</sub> [3] chain-like candidate, which may host a similar bond-nematic state within a narrow magnetic field range around 40 T and just below saturation, in our model,

this novel order appears at a magnetic field that is 1/3 of its saturation value, which is much lower than 40 T. The model considered may underpin a more experimentally accessible alternative to study and observe the long sought spin nematic order

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## Stability and Fluctuation of Snake-like Magnetic Domains in Kagome Spin Ice.

Wen-Han Kao (National Taiwan University), Ying-Jer Kao (National Taiwan University)

We study the two-dimensional kagome ice system with canted spins pointing into the easy directions of pyrochlore spin ice. With these canted spins, out-of-plane magnetic field can be used for tuning the density of magnetic charges. It was reported that an in-plane magnetic field can lead to a two-stage magnetization process in 2D dipolar kagome ice [1] and a special q = X long-range ordered state in 3D dipolar pyrochlore spin ice [2]. By using this two-component external field and spin-spin interaction beyond second-nearest-neighbor level, we discuss the competition among different possible ground states and new emergent phenomena in this system. In the phase boundary of known ground states, we found a new metastable nematic state formed by snake-like domains which are energetically more favored than conventional loop or string excitations. By analyzing the excitation energy and interfacial free energy, we explain the origin of these long-lived domains and propose possible updates in the simulation to enhance domain fluctuations. Finally, the topological bottleneck in the relaxation process is studied through the waiting time Monte Carlo method [3].

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Crystal Structure and Quantum Magnetism of Spin-1/2 Triangular-Lattice Antiferromagnet Ba<sub>2</sub>La<sub>2</sub>CoTe<sub>2</sub>O<sub>12</sub>.

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Y. Kojima(Tokyo Inst. of Tech.), M. Watanabe(Tokyo Inst. of Tech.), N. Kurita(Tokyo Inst. of Tech.), H. Tanaka (Tokyo Inst. of Tech.), A. Matsuo(ISSP, Univ. Tokyo) and K. Kindo(ISSP, Univ. Tokyo) —

Spin-1/2 triangular-lattice antiferromagnet (TLAF) is a typical frustrated quantum magnet. Great effort has been made to explore the nature of their ground state and magnetic excitations. On the experimental side, many materials have been developed as candidates of spin-1/2 TLAFs. Ba<sub>2</sub>La<sub>2</sub>CoW<sub>2</sub>O<sub>12</sub> is known to have a uniform triangular lattice of Co<sup>2+</sup> with effective spin-1/2 [1]. However, the nearest-neighbor (NN) exchange interaction was found to be ferromagnetic and weak [2,3]. Because the filled outermost orbitals of W<sup>6+</sup> is 5p, it is considered that the antiferromagnetic superexchange interaction via Co<sup>2+</sup>-O<sup>2-</sup>-O<sup>2-</sup>-Co<sup>2+</sup> and the ferromagnetic superexchange interaction via

 $Co^{2+}-O^{2-}-W^{6+}-O^{2-}-Co^{2+}$  almost cancel out [4,5]. If  $W^{6+}$  is replaced with  $Te^{6+}$  that has the filled outermost orbitals of 4d, the superexchange interaction via  $Co^{2+}-O^{2-}-Te^{6+}-O^{2-}-Co^{2+}$  should be antiferromagnetic.

Consequently, the NN exchange interaction will be antiferromagnetic and strong. In this study, we synthesized  $Ba_2La_2CoTe_2O_{12}$ , which has the same crystal structure as  $Ba_2La_2CoW_2O_{12}$ , and investigated its magnetic properties using powdered sample. It was found from the temperature dependence of magnetic susceptibility and specific heat that  $Ba_2La_2CoW_2O_{12}$  has the antiferromagnetic NN exchange interaction and undergoes magnetic ordering at  $T_N=3.2~\rm K$ . The magnetization curve exhibits a plateau at one-third of the saturation magnetization, which is characteristic of triangular-lattice quantum antiferromagnet.

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## Frustration effects in the magnetic dynamics above $T_N$ in h-YMnO<sub>3</sub>.

J. Lass, S. Janas, S. Holm-Dahlin, L. Ø. Sandberg, M. L. Haubro, T. K. Schäffer (Univ. Cph.); A. Fennell, U. Stuhr (Paul Scherrer Inst.); Z. Yamani (Chalk River Nat. Lab.); A. Schneidewind (Research Center Jülich); Zhilun Lu (Helmholtz Center Berlin); D. Prabhakaran (Univ. Oxford), and K. Lefmann (Univ. Copenhagen) —

The hexagonal manganite h-YMnO<sub>3</sub> is much studied for its multiferroic properties, where spin and lattice degrees of freedom are intertwined [1]. However, the magnetic subsystem of the material is also strongly frustrated ( $f \approx 7$ ), as it is

a close realization of a 2D antiferromagnet on the triangular lattice [2]. We have studied the magnetic dynamics of h-YMnO<sub>3</sub> with neutron scattering and found a strong, inelastic diffuse signal appearing at the magnetic zone boundary, indicating magnetic fluctuations in the range 1-10 meV with a correlation length of 2-3 nm. Polarized inelastic neutron scattering confirms this signal to be magnetic. The signal strongly increases with temperature just below  $T_N = 72$  K, but then remain almost constant up to around 200 K, where the correlation length starts decreasing. The q-dependence of the inelastic signal reflects the underlying hexagonal lattice symmetry, not unlike what is found for jarosite [3]. The modulation vector of this signal differs strongly from that of the ordered state, and we believe to have observed a transition from 3D ordering to 2D short range order, much below the Curie-Weiss temperature of the material. At the conference, we will present a detailed analysis of the recent data from the point of view of classical antiferromagnetic spin dynamics on the 2D triangular lattice.

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## Magnetic analogue of the Haldane model

C. Lee (OIST), J. Romhányi (OIST), and N. Shannon (OIST) —

Haldane's model of electrons with complex hopping on the honeycomb lattice provides one of the simplest examples of how topological order can enter into the bandstructure of a material [1]. Realising this model using electrons, however, proves challenging, and the question of whether equivalent effects exist in the bandstructure of bosonic magnetic excitations poses interesting possibilities. Here we show how a realistic model of a ferromagnetic insulator with a spin-orbit coupling can achieve the magnetic analog of the Haldane model on the honeycomb lattice. Starting from a ferromagnetic state, we find well—defined bands of magnon excitations with non–trivial Chern numbers, implying that the magnetic model also exhibits chiral edge states and an anomalous thermal Hall effect. These results confirm that magnets can realize many of the effects reported in topological insulators and semi-metals.

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## Competing phases and topological excitations of spin-one pyrochlore antiferromagnets.

F.-Y. Li (Fudan Univ.) and G. Chen (Fudan Univ.)

Most works on pyrochlore magnets deal with the interacting spin-1/2 local moments. We here study the spin-one local moments on the pyrochlore lattice, and propose a generic interacting spin model on a pyrochlore lattice. Our spin model includes the antiferromagnetic Heisenberg interaction, the Dzyaloshinskii-Moriya interaction and the single-ion spin anisotropy. We develop a flavor wave theory and combine with a mean-field approach to study the global phase diagram of this model and establish the relation between different phases in the phase diagram. We find the regime of the quantum paramagnetic phase where a degenerate line of the magnetic excitations emerges in the momentum space. We further predict the critical properties of the transition out of the quantum paramagnet to the proximate orders. The presence of quantum order by disorder in the parts of the ordered phases is then suggested. We point out the existence of degenerate and topological excitations in various phases. We discuss the relevance with fluoride pyrochlore material NaCaNi<sub>2</sub>F<sub>7</sub> and explain the role of the spin-orbit coupling and the magnetic structures of the Ru-based pyrochlore A<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub> and the Mo-based pyrochlore A<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub>.

arXiv:1712.00740

## Projective symmetry group classification of $Z_2$ spin liquids in a pyrochlore lattice.

C. Liu (UCSB), G. Halász (KITP), and L. Balents (KITP)

The rare-earth pyrochlore oxides  $R_2M_2O_7$  are a class of compounds that supports frustrated magnetism, and some of them are predicted to host a spin liquid state in presence of strong quantum effects. Propelled by this theoretical idea and recent experimental observations, we give a complete classification of  $Z_2$  spin liquid states in the pyrochlore lattice formed by the rare earth R ions within the projective symmetry group approach. A list of mean field states is given to

match the classically ordered phases, and the transitions into spin liquid states are analyzed. The effects of strong spin-orbit coupling in the pyrochlore materials are also discussed. This study provides a clear map of phases of pyrochlore for future experiments and further variational Monte-Carlo study of the spin liquid states in pyrochlore materials.

## Extended Coulomb liquid phase of a generic hardcore boson model on a pyrochlore lattice.

C. Liu(Fudan Univ.), C.-J. Huang(USTC), Z. Y. Meng(ITP CAS), Y. Deng(USTC) and G. Chen(Fudan Univ.) — Motivated by the growing activities in the U(1) Coulomb liquid, we explore the phase diagram of a paired hardcore boson model on the pyrochlore lattice. Unlike the usual hardcore boson model with only boson hopping and interaction, this model contains an extra boson pairing term. This model is equivalent to the XYZ spin model that was proposed for certain rare-earth pyrochlore materials [1,2]. Since it was proposed that this model has no sign problem in a large parameter regime for quantum Monte Carlo simulations [2], we carry out both analytical and quantum Monte Carlo calculation and obtain a consistent phase diagram. It is found that the U(1) Coulomb liquid is stable and spans a large portion in the parameter space with the introduction of the boson pairing. Moreover, we find numerical evidence that the boson pairing could induce a fully-gapped Z2 liquid in the vicinity of the phase boundary between Coulomb liquid and the ferromagnetic spin order in the spin language. Apart from the materials' relevance that was proposed previously, we point out the quantum simulation with cold atoms and ion crystals.

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## Robustness of frustration and spin origami/kirigami in the kagome Fluorides.

Michael J. Lawler (Cornell U., Binghamton U.), Krishanu Roychowdhury (Cornell U.) and D. Zeb Rocklin (Georgia Tech, Cornell U.)

We study the robustness of frustration in kagome antiferromagnets under a distortion of the lattice as exemplified by the fluoride materials. Assuming nearest neighbor couplings continue to dominate the physics, we show that ground states are in general a triangulated surface with spins lying on the edges. If the surface has no holes in it, we call such a state spin origami and if it has holes spin kirigami. We identify a simple criterion to distinguish whether a give material has spin origami or spin kirigami ground states. Focusing on origami materials, we compute these ground states for  $Cs_2ZrCu_3F_{12}$  and  $Cs_2CeCu_3F_{12}$  and show the former has a flattenable origami ground state while the latter a non-flattenable origami. We further derive a topological invariant which governs the spin waves spectra of any spin origami building on recent developments in our understanding of Maxwell counting[1,2]. It demands a flat band for the flattenable case and topological (Weyl) lines of zero modes in the nonflattenable case. For  $Cs_2CeCu_3F_{12}$ , symmetry enhances the topology and demands line nodes are doubly degenerate (i.e., Dirac line nodes). These results suggest topological invariants could similarly be used to capture the origin of frustration in a variety of magnets.

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## Possible quadrupolar nematic phase in the frustrated spin chain LiCuSbO<sub>4</sub>: an NMR investigation

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The frustrated one-dimensional (1D) quantum magnet LiCuSbO<sub>4</sub> is one rare realization of the  $J_1 - J_2$  spin chain model with an easily accessible saturation field, formerly estimated to 12 T [1]. Exotic multipolar nematic phases are theoretically predicted for such spin chains just below the saturation field, but without unambiguous experimental observation so far. We present an extensive experimental research on this compound in the wide temperature

(30 mK-300 K) and field (0-13.3 T) range by muon spin rotation (μSR), <sup>7</sup>Li nuclear magnetic resonance (NMR) on *oriented* samples and magnetic susceptibility (SQUID). μSR experiments in zero magnetic field demonstrate the absence of long range 3D ordering down to 30 mK. Together with former heat capacity data [1], magnetic susceptibility measurements suggest a short range correlated vector chiral phase in the field range 0 – 4 T. In the intermediate field values (5-12 T), the system enters a 3D ordered spin density wave phase with 0.75 μ<sub>B</sub> per copper site at the lowest temperature (125 mK), estimated by NMR. At still higher field, the magnetization is found to be saturated above 13 T where the spin lattice T<sub>1</sub><sup>-1</sup> relaxation reveals a spin gap estimated to 3.2(2) K. We sketch a phase diagram where we narrow down the possibility of observing a multipolar nematic phase to the range 12.5-13 T [2]. These results are discussed in view of the theoretical phase diagram of ref.[3], related theory papers and a concomitant work by the Dresden NMR group [4].

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#### Quantum Phase Diagram of Frustrated Spin-1/2 System on a Trellis lattice.

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Recently synthesized compounds like SrCu<sub>2</sub>O<sub>3</sub>, LaCuO<sub>2·5</sub>, MgV<sub>2</sub>O<sub>5</sub> have the effective interactions limited only to two dimensional trellis lattice, and this system shows a weak ferromagnetic coupling [1,2,3]. This system displays evidently the presence of spin-gap even in weak rung interaction. In our numerical studies we show the existence of many exotic phases like incommensurate spiral, decoupled, dimer and short range order phases. The spin-spin correlation functions in the incommensurate phase follow power law decay in contrary to exponential behavior of correlations in frustrated quasi 1D systems [4, 5]. We also study different exchange coupling dependences of pitch angle in incommensurate spiral regime.

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#### Magnons in a Strongly Spin-Orbital Coupled Magnet.

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We present the non-linear spin-wave theory calculations of the dynamical response of an extended Kitaev-Heisenberg model for the parameters applicable to  $\alpha$ -RuCl<sub>3</sub>. We argue that large anisotropic terms of spin-orbit nature necessarily imply strong anharmonic coupling of magnons. Subsequently, the overlap of one- and two-magnon states must lead to broad spectral features in magnon spectrum. These are accompanied by a significant longitudinal component of the structure factor from the two-magnon states that are also broadened. We calculate magnon decay rates due to anharmonic coupling within a self-consistent approach and find our results for the dynamical structure factor to be in a good agreement with both exact diagonalization results for the same set of parameters and experiment.

## Asymmetric melting of one-third plateau in kagome quantum antiferromagnets

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Asymmetric destruction of the one-third magnetization plateau upon heating is found [1] in the spin-1/2 kagome Heisenberg antiferromagnets using the typical pure quantum state approach. The asymmetry originates from larger density of states of low-lying excited states of  $N_{\rm s}$  spin systems with magnetization  $(1/3-2/N_{\rm s})$  than that of low-lying

states with magnetization  $(1/3 + 2/N_s)$ . The enhanced specific heat and entropy that reflect the larger density of states in the lower-field side of the plateau are detectable in candidate materials of the kagome antiferromagnets. We discuss that the asymmetry originates from the unprecedented preservation of the ice rule around the plateau. A part of calculations is done by using open-source software  $\mathcal{H}\Phi$  [2,3].

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## Interaction effects on the Kane-Mele Model in the Hofstadter regime.

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Considering interacting Kane-Mele model of honeycomb lattice in the Hofstadter regime, we realize that the orbital motion of electrons can induce versatile topological phases with spontaneously broken symmetries. In the Hofstadter regime without spin orbit coupling, the interactions lead to the breaking of translational and rotational symmetries of the system resulting in nematic and ferrielectric phases [?, ?]. Here, within the mean field framework, we extend the study and consider the onsite and nearest neighbor interactions in the Kane-Mele model and discuss possible phases in the absence and presence of magnetic field at each integer filling of electrons.

- 1. Interaction effect on Kane Mele model at zero magnetic field: At half filling, the interplay of intrinsic spin-orbit coupling and onsite interaction leads to the phase transition from quantum spin Hall insulator to an antiferromagnetic Mott insulator with magnetization in the *xy*-plane. At quarter filling, we study this interplay and show that the combined effect opens a wide region of ferromagnetic Chern insulating phase in between metal and normal insulator. We further discuss the experimental realization of these phases in series of transition metal trichalcogenides [?].
- 2. We extend our study to analyze the collaborative effect of magnetic field, spin orbit coupling and interactions. Focusing on  $2\pi/3$  magnetic flux per plaquette, we realize numerous interesting phases like insulator with noncoplanar magnetic ordering, ferrimagnetic Chern insulator with nematic charge order, ferrimagnetic-ferrielectric Chern insulators etc. Many of these phase transitions are also accompanied with the change in the topology of the system. Our theoretical study broadens the field of topological phases accompanied with multiferroic like properties, as a consequence of the interplay of magnetic field, spin orbit coupling and interactions [?].

# Machine learning meets quantum spin-dynamics: improving the resolution of the dynamical spin structure factor in tDMRG calculation.

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Dynamical spin structure factor is one of the most important quantities that bridge between experimental data and theoretical calculation in condensed matter physics. Recently, it has become possible to calculate it by time-dependent DMRG (tDMRG) calculation with matrix product states (MPS)[1], which is based on obtaining the two-time correlators by time evolution of the wavefunction and subsequent Fourier transform. Among various efforts made to archive the better resolution in faster computation time, the application of the linear prediction in order to extend the time-dependent signal to the larger time has gained the popularity [2]. Motivated by the same philosophy, this work explores various different machine learning techniques to improve the resolution and benchmarks each method using spin-1/2 XXZ model in 1D as a playground.

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## SU(4)-symmetric spin-orbital liquids on the hyperhoneycomb lattice

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The search for exotic states of matter induced by the combined effects of strong correlation and spin-orbit coupling has stimulated the study of transition metal oxides with 4d and 5d elements. We have developed theoretical tools to describe the magnetism of these compounds when the heavy ion is in the  $d^1$  configuration in previous works [?, ?]. In the present work, we study the effective spin-orbital model that describes the magnetism of 4  $d^1$  or 5  $d^1$  Mott insulators in ideal tricoordinated lattices [?]. The model is displays anisotropic and bond-dependent interactions between multipoles of j=3/2 angular moment operators. However, in the limit of vanishing Hund's coupling, the model has an emergent SU(4) symmetry. We demonstrate that this large symmetry can be made explicit by means of a Klein transformation on pseudospin degrees of freedom. A geometrical criterion for the emergence of this SU(4)-invariance was proposed. Taking the hyperhoneycomb lattice as an example, we employ parton constructions with fermionic representations of the pseudospin operators to investigate possible quantum spin-orbital liquid states. The energies of the projected wave functions were computed using variational Monte Carlo methods. Our numerical results show that the lowest-energy quantum liquid corresponds to a zero-flux state with a Fermi surface of four-color fermionic partons.

## Degenerate ground state in classical pyrochlore antiferromagnet Na<sub>3</sub>Mn(CO<sub>3</sub>)<sub>2</sub>Cl

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A classical pyrochlore antiferromagnet exhibits neither a magnetic order nor spin glass because of an infinite degeneracy in a ground state[1, 2]. Na<sub>3</sub>Mn(CO<sub>3</sub>)<sub>2</sub>Cl is a new candidate for a classical pyrochlore antiferromagnet, where a pyrochlore network of S = 5/2 is formed by MnO<sub>6</sub> octahedra linked by carbonate ions. Because of the high isotropy in spin interactions, Na<sub>3</sub>Mn(CO<sub>3</sub>)<sub>2</sub>Cl exhibits largely different magnetic properties from those of the Co-analogue, Na<sub>3</sub>Co(CO<sub>3</sub>)<sub>2</sub>Cl[3], which exhibits an all-in-all-out order at 1.5 K. The temperature dependence of the magnetic susceptibility and the magnetization curves are consistent with those of a S = 5/2 pyrochlore lattice antiferromagnet with nearest-neighbor interactions of 2 K. No signature of a spin-glass was observed in the temperature dependence of the ac-susceptibility above 2 K, and no Bragg peak indicating a magnetic order was detected in powder neutron diffraction measurements collected at 0.05 K using ECHIDNA diffractometer. On the other hand, enhancement of an antiferromagnetic short range order is evidenced by the diffuse scattering which develops around 0.85 Å<sup>-1</sup>. Analyses based on a mean-field theory[4] supports that its Q-dependence is due to dominant nearest-neighbor antiferromagnetic interactions. In addition, from heat capacity measurements, the magnetic entropy of 4 J K<sup>-2</sup> mol<sup>-1</sup>, which corresponds to 1/4 of the total entropy, is likely to persist even at 0.5 K. Thus, a large degeneracy should be present near a disordered ground state in Na<sub>3</sub>Mn(CO<sub>3</sub>)<sub>2</sub>Cl.

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### Mott transition in the pyrochlore oxides.

N. Swain(NTU, Singapore) and P. Majumdar(HRI, India) —

We study the interplay of electron correlation and geometric frustration in the context of the Mott transition in the pyrochlore lattice. We formulate the single band Hubbard model on this lattice in terms of electrons coupled to auxiliary local magnetic moments, and treat the resulting 'fermion-spin' problem through a real space Monte Carlo technique. While the ground states we obtain are equivalent to unrestricted Hartree-Fock, the presence of crucial low energy fluctuations in our approach, and their coupling to the electrons, allows us to establish the temperature dependence of transport and spectral features across the Mott transition. Our study shows the pyrochlore lattice has no long-range ordered state. In the vicinity of the Mott transition, the local moments become small and the coupling of electrons to

these leads to an anomalous resistive state. We further attempted to model the more complex and experimentally relevant pyrochlore molybdates and iridates by including Hund's and spin-orbit coupling respectively. We have thoroughly studied the model problems and have obtained the overall phase diagrams capturing the details of the Mott transition observed in the pyrochlore molybdates and iridates.

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## Competing Phases in the Quantum S=1/2 ANNNH Model.

J. Oitmaa (UNSW, Sydney, Australia) and R.R.P. Singh (UC Davis) —

The S=1/2 antiferromagnet with frustration arising from second-neighbor coupling in one axial direction only (the ANNNH model) is studied via series methods at T=0 and at high T. We find an incommensurate spiral phase at T=0 in two dimensions, extending to finite temperatures in three dimensions. A conjectured modulated collinear phase is found to have a substantially higher energy and hence is not realized in this model.

## Frustrated $J_1$ - $J_2$ - $J_3$ Heisenberg Antiferromagnet on the Simple Cubic Lattice.

J. Oitmaa (UNSW, Sydney, Australia) —

The frustrated  $J_1$ - $J_2$ - $J_3$  antiferromagnet on the smple-cubic lattice shows three types of AF order. A recent functional renormalization group calculation has predicted an intermediate disordered phase at zero temperature near the point of maximum frustration. Series expansions for S=1/2 show signs of such a disordered phase, albeit over a smaller region of the phase diagram.

## Nature of Ba<sub>3</sub>MIr<sub>2</sub>O<sub>9</sub> (M=Sc,Y,In) ground state probed by $\mu$ SR.

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The search for quantum spin liquid states, such as the resonant valence bond state formed by the macroscopic resonance between the various spin singlet coverings of the lattice, is a major challenge in both experimental and theoretical condensed matter research [1]. Nevertheless, the key feature to stabilize such a ground state, i. e. the magnetic frustration, is not sufficient in the triangular case [2]. Therefore, to destabilize the ordered ground state one has to implement a deviation from this model such as a lower coordination number in the kagome model [3], or the introduction of spin-orbit coupling (SOC) [4].

We present here our  $\mu$ SR study on some compounds of the Ba<sub>3</sub>MIr<sub>2</sub>O<sub>9</sub> family which offers a tremendous playground to study the influence of this latter. The magnetism in these materials is based on iridium dimers which are set on a bidimensional triangular lattice [5]. Further, by changing the non-magnetic ion M one can tune the effective value of the dimers spin J. In this presentation we will focus on the J=1/2 compounds (M=Y, Sc, In) which present all the characteristics to stabilize a quantum spin liquid ground state.

We did zero field measurements in order to probe the nature of the ground state in the different compounds. For the Y and Sc ones we found an homogeneous ordered ground state, with transitions at 4.5 K and 10 K respectively, as expected from the susceptibility, heat capacity and NMR measurements [6]. On the contrary, for the In one, we found no sign of frozen magnetism down to 20 mK despite interactions of about 130 K, which could be the sign of a spin liquid ground state. Moreover, our transverse field measurements point out a local susceptibility for the muon similar to our squid and NMR experiments, enlightening the absence of defects. In addition, our NMR and heat capacity measurements are in favor of a gapless spin liquid ground state [7]. Understanding the mechanisms which drive the ordering of the magnetism could help to have a better insight on how to stabilize a quantum spin liquid ground state.

To address this issue, one can think of three different explanations. First, a first principle calculation study on the Y compound pointed out the stabilization of an ordered ground state due to a small SOC value in regard to the Heisenberg

interaction. However, as each studied samples present the same lattice and effective spin one could expect a similar ratio between the SOC and the Heisenberg interaction. Nevertheless, a small variation in the SOC coupling value could lead to a quite different ground state. Second, a more careful study of the interactions between the Ir dimers enlighten two interactions,  $J_T$  in the (ab) plane and  $J_H$  along the (c) direction. We propose that the ratio among  $J_H$  and  $J_T$  drives the transition from an ordered ground state to a spin liquid one. Indeed, the Y and Sc compounds magnetism could be modeled by a triangular lattice ( $J_T \ll J_H$ ) whereas a more complex model with a mix between honeycomb and triangular lattice ( $J_T \propto J_H$ ) has to be taken into account for the In material. Last, there could be an influence of the orbitals in game in the superexchange coupling. Indeed, the Sc<sup>3+</sup> and Y<sup>3+</sup> ions present a fully occupied valency orbital p whereas the In<sup>3+</sup> ions possess a fully occupied valency orbital p. In the perspective, we propose different theoretical and experimental investigations to address those hypothesis.

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## $\mu$ SR study of a S=1 kagome compound.

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(Uni St-Andrews), R.E. Morris (Uni St-Andrews), A. Amato (PSI), C. Baines (PSI) and F. Bert (Uni Paris-Sud) — The study of the Kagome antiferromagnetic model (KAFM) has lately focused on the quantum (S=1/2) [1] and on the classical (S>1) [2] cases. The intermediate case, S=1, has been poorly studied. An exotic ground state, a valence bond crystal, is expected to be stabilized but the pattern of the crystal, hexagonal or trimerized [3] is still theoretically debated.

On the experimental side, only few compounds have been synthesized. The most studied one, m-MPYNN.BF<sub>4</sub>, does not exhibit any sign of frozen magnetism down to 30 mK despite an antiferromagnetic interaction of -3 K. Further, some heat capacity and susceptibility measurement have evidenced a gap in the excitation spectrum but no strong evidence on favor of the hexagonal or trimerized pattern has been found [4].

Recently, F. H. Aidoudi *et al.* synthesized a KAFM S=1 compound based on  $V^{3+}$ ,  $(NH_4)_2[C_2H_8N][V_3F_{12}]$  [5]. Their magnetic susceptibility measurements point out two transitions at 10 K and 6 K despite a Curie Weiss temperature of -28(2) K, leading to an antiferromagnetic long range ordered (AFLRO) or a spin glass like ground state.

In order to have a better characterization of the ground state, we performed  $\mu$ SR and heat capacity experiments without applied field. The  $\mu$ SR study unveils an exotic magnetic behavior with two transitions. The first one occurs at 10 K and is characteristic of a transition to a frozen state without long range ordering. The second one occurs at 6 K and points out a transition to a mixed ground state with coincidence of incommensurate AFLRO part and glassy part. The heat capacity measurements reveal only a peak at 10 K. Further, the residual entropy below 10 K is rather small (20 % of the total one). This is characteristic of a freezing of the degree of freedom above the 10 K transition [6].

Therefore, we argue that the 10 K transition is related to a ferromagnetic ordering of the spin part perpendicular to the kagome lattice which is certainly due to anisotropies. By analyzing the value of the weak ferromagnetism it seems that it cannot be only related to the Dzyaloshinskii Moryia interaction [7] but may involve also the distortion of the lattice or on-site anisotropy. Then, the 6 K transition could be related to the ordering of the spin part parallel to the kagome planes leading to a three dimensional ordered or glassy magnetism. Some neutron experiment as well as DFT calculations could help to understand the incommensurability of the magnetic lattice at base temperature.

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## Entanglement in the One-Dimensional SU(2) ⊗SU(2) Models.

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In insulating states of transition metal oxides with orbital degeneracy effective interactions are described in terms of spin-orbital superexchange [1]. Consequently, the resulting models are often inherently frustrated and the quasi-empirical Goodenough-Kanamori rules may be violated leading to (intersite) spin-orbital entanglement which excludes the use of mean field procedure separating spin and orbital degrees of freedom [2]. In this talk we first give a brief overview of the earlier study of the one-dimensional (1D) SU(2) $\otimes$ SU(2) symmetric models that show entangled spin-orbital bound states and enhanced spin-orbital fluctuations, both for antiferromagnetic and ferromagnetic exchange [3], and analyze the respective phase diagrams. We show that in general spin-orbital fluctuations are enhanced near the highly symmetric SU(4) model. Next, we concentrate on a 1D spin-orbital model with lower symmetry, that, however, is able to describe a wider class of transition metal oxides [4]. It turns out that, even though such a model exhibits a more complex spin-orbital entanglement, amazingly it can under some circumstances be reduced to an exactly solvable free fermion model. This property gives more insights into the nature of spin-orbital correlations.

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## Emergent spin-1 Haldane gap and ferroelectricity in a frustrated spin-1/2 ladder Rb<sub>2</sub>Cu<sub>2</sub>Mo<sub>3</sub>O<sub>12</sub>.

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The quasi-one-dimensional magnet Rb<sub>2</sub>Cu<sub>2</sub>Mo<sub>3</sub>O<sub>12</sub> [1] shows both a spin gap and a ferroelectricity stabilized by a magnetic field [2,3]. However, the relation between the magnetism and the ferroelectricity remains open, and the material has been a candidate for a novel prototype of multiferroics that hosts a ferroelectricity induced by a vector spin chirality in the absence of a long-range magnetic order. Here we report its combined experimental and theoretical evidence by means of polarization, thermodynamic, inelastic neutron-scattering, electron spin resonance measurements as well as extensive theoretical analyses of frustrated spin-1/2 chains involving ferromagnetic first-neighbor and antiferromagnetic second-neighbor exchange interactions. It has already been known that nontrivial ground states appear in the single frustrated chain, where spin-singlet short-range resonating valence bonds connect emergent spin-1 pairs with and without a spontaneously broken parity due to a vector spin chirality order [4-6]. Our analyses uncover that the non-magnetic ground state of Rb<sub>2</sub>Cu<sub>2</sub>Mo<sub>3</sub>O<sub>12</sub> is described by effective spin-1 pairs forming a tetramer singlet ground state with the Haldane spin gap in a frustrated spin-1/2 two-leg ladder model. Although a splitting of the spin-1 triplet excitations into three by alternating Dzyloshinskii-Moriya interactions is observed with our neutron-scattering and electron resonance spectra and explained by the current theory, we have found that the ground state is adiabatically connected to that of the decoupled spin-1 Haldane chains.

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## Spin Dynamics of the Molecular Frustrated System EtMe<sub>3</sub>Sb[Pd(dmit)<sub>2</sub>]<sub>2</sub> investigated by ESR measurements

Y. Oshima (RIKEN), S. H. Kim (Hokkaido Univ.) and R. Kato (RIKEN)

The anion radical salts  $X[Pd(dmit)_2]_2$  (X is a monovalent cation) are Mott insulators which consist of S=1/2 triangular lattice. The fascinating feature of this sytem is that the geometrical frustration of the triangular lattice can be tuned by substituting the cation X, and a wide variety of magnetic ground state can be observed [1,2]. The  $X=EtMe_3Sb$  salt shows no long range-order down to 19 mK, and it is considered as a strong candidate material for the quantum spin liquid (QSL) state. However, the nature of its low-lying elementary spin excitation and the presence or the absence of a spin-gap is still under strong debate. Electron spin resonance (ESR) is one of the sensitive probes that can provide microscopic information of the local environement surrounding the electron spins, and it has the potential to directly observe the elementary excitations of the QSL state and studying its properties. Hence, we present our ESR results on the QSL material  $EtMe_3Sb[Pd(dmit)_2]_2$ , and reveal its spin correlations and spin dynamics.

When the magnetic field is rotated parallel to the triangular lattice, two ESR absorption lines were observed. From the angular dependence of the *g*-value, these ESR absorptions are from the Pd(dmit)<sub>2</sub> dimers in two independent layers where the dimer stacking directions are different. In turn, such observation of two ESR lines suggests the interlayer exchange interaction is infinitesimal, estimated ca. 0.37 mK, which is in good agreement with the absence of long-range order. Furthermore, the ESR linewidth shows a characteristic and continuous narrowing down to the lowest temperature, and the power dependence shows a peculiar feature that is not observed for analog salts with different ground states. We suppose that ESR is probing the elementary excitations of the QSL state known as the spinon, and the narrowing of the ESR linewidth suggests that spinons in this system are highly mobile. Moreover, a peculiar angular dependence of linewidth, which can be attributed to a quasi-1D spin diffusion are obsevred. This indicates that the spin dynamics of the spinon is quite anisotropic despite that the system have a triangular magnetic network.

In our presentation, the characteristic ESR behavior of EtMe<sub>3</sub>Sb[Pd(dmit)<sub>2</sub>]<sub>2</sub> will be presented, and the ESR results will be compared with the anolog Pd(dmit)<sub>2</sub> salts with antiferromagnetic (Me<sub>4</sub>P[Pd(dmit)<sub>2</sub>]<sub>2</sub>), charge ordered (Et<sub>2</sub>Me<sub>2</sub>Sb[Pd(dmit)<sub>2</sub>]<sub>2</sub>), and valence bond solid (EtMe<sub>3</sub>P[Pd(dmit)<sub>2</sub>]<sub>2</sub>) ground state. Although the ground state is non-magnetic with a spin gap of about 90 K, the excited state of the valence bond solid material seems to also have a quasi-1D spin dynamics.

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## Quantum Dynamics in Kagome Ice Ho<sub>3</sub>Mg<sub>2</sub>Sb<sub>3</sub>O<sub>14</sub>

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A promising route to realize entangled magnetic states combines geometrical frustration with quantum tunneling effects. Spin-ice materials are canonical examples of frustration [1], and Ising spins in a transverse magnetic field are the simplest many-body model of quantum tunneling [2]. In this talk, I will show that the tripod kagome-lattice [3,4] material  ${\rm Ho_3Mg_2Sb_3O_{14}}$  unites an ice-like magnetic degeneracy with quantum-tunneling terms generated by an intrinsic splitting of the  ${\rm Ho^{3+}}$  ground-state doublet. I present neutron-scattering and thermodynamic data that reveal a symmetry-breaking transition at  $T^*\approx 0.32~{\rm K}$  to a state with three remarkable features: persistent spin fluctuations down to  $T\approx 0.12~{\rm K}$ ; a macroscopic degeneracy of ice-like microstates; and a fragmentation of the spin into periodic and aperiodic components [4]. I discuss a model incorporating the interplay of frustration and quantum dynamics that explains our scattering data. Our results establish that  ${\rm Ho_3Mg_2Sb_3O_{14}}$  realizes quantum kagome ice, a frustrated Ising model with an intrinsic transverse field.

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# Single crystal growth of $\text{Cu}_4(\text{OH})_6\text{BrF}$ and universal behavior in quantum spin liquid candidates synthetic barlowite and herbertsmithite.

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Synthetic barlowite,  $Cu_4(OH)_6BrF$ , contains kagomé layers of S=1/2  $Cu^{2+}$  ions separated by interlayer  $Cu^{2+}$  ions. Substitution of the interlayer  $Cu^{2+}$  ions with  $Zn^{2+}$  ions has been reported to induce a quantum spin liquid (QSL) ground state similar to synthetic herbertsmithite,  $ZnCu_3(OH)_6Cl_2$ . Here we discuss a scalable synthesis of single crystals of  $Cu_4(OH)_6BrF$  which can be extended to  $ZnCu_3(OH)_6BrF$ . Using a number of diffraction techniques coupled with magic angle spinning NMR spectroscopy, we resolve the previously reported positional disorder of the interlayer  $Cu^{2+}$  site and find that the structure is best described in the orthorhombic space group, Cmcm, with an ordered arrangement of interlayer  $Cu^{2+}$  ions. Infrared spectroscopy measurements of the O-H and F-H stretching frequencies demonstrate that the orthorhombic symmetry persists upon substitution of  $Zn^{2+}$  for  $Cu^{2+}$  on the interlayer site. Specific heat and magnetic susceptibility measurements of Zn-substituted barlowite,  $Zn_xCu_{4-x}(OH)_6BrF$ , reveal striking similarities with the behavior of  $Zn_xCu_{4-x}(OH)_6Cl_2$ . These parallels imply universal behavior of copper kagomé lattices even in the presence of small symmetry breaking distortions. Thus synthetic barlowite demonstrates universality of the physics of synthetic  $Cu^{2+}$  kagomé minerals and furthers the development of real QSL states.

### Magnetic field-induced evolution of intertwined orders in the Kitaev magnet $\beta$ -Li<sub>2</sub>IrO<sub>3</sub>.

N. Perkins (U. Minnesota) —

Recent scattering experiments in the 3D Kitaev magnet  $\beta$ -Li<sub>2</sub>IrO<sub>3</sub> have shown that a relatively weak magnetic field along the crystallographic b-axis drives the system from its incommensurate counter-rotating order to a correlated magnet, with a significant uniform zigzag component superimposing the magnetization along the field. Here it is shown that the zigzag order is not emerging from its linear coupling to the field (via a staggered, off-diagonal element of the g-tensor), but from its intertwining with the incommensurate order and the longitudinal magnetization. The emerging picture explains all qualitative experimental findings at zero and finite fields, including the rapid decline of the incommensurate order with field and the so-called intensity sum rule. The latter are shown to be independent signatures of the smallness of the Heisenberg exchange J, compared to the Kitaev coupling K and the off-diagonal anisotropy  $\Gamma$ . Remarkably, in the regime of interest, the field  $H^*$  at which the incommensurate component vanishes, depends essentially only on J, which allows to extract an estimate of  $J \simeq 4K$  from reported measurements of  $H^*$ . We also comment on recent experiments in pressurized  $\beta$ -Li<sub>2</sub>IrO<sub>3</sub> and conclude that J decreases with pressure.

#### Sc doping near the quantum critical point in weak antiferromagnetic TiAu.

M. Mathew (UC Davis), W. F. Goh (U. C. Davis) and W. E. Pickett (UC Davis) —

The weak antiferromagnetism (wAFM) of TiAu, [1] a compound comprised of two non-magnetic elements, has been accounted for in previous work [2,3] as arising not from nested Fermi surfaces as is commonly discussed for wAFMs, but from mirrored van Hove singularities. The latter mechanism involves smaller volumes of the Brillouin zone and different characteristics of the Fermi surface (FS): small electron velocities around a topological change in the FS, versus large areas of parallel FS for the nesting scenario. Here we address real space behavior arising from hole (Sc) doping on the Ti sublattice, which disturbs the electronic and magnetic structure as well as lowering the Fermi level relative to the magnetic Ti 3d states. The manner in which Sc atoms alter the electronic spectrum and disturb the magnetism, whether by annihilating Ti moments or frustrating coupling of surviving moments, will be presented and analyzed.

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#### Dynamic quantum kagome ice.

S. Petit (Laboratoire Léon Brillouin, France), E. Lhotel (Institut Néel, France), M. Ciomaga Hatnean (University of Warwick, United Kingdom), J. Ollivier(Institut Laue Langevin, France), H. Mutka (Institut Laue Langevin, France), E. Ressouche (CEA Grenoble, France), M. R. Lees (University of Warwick, United Kingdom), G. Balakrishnan (University of Warwick, United Kingdom)

In spin ice physics, although different at first glance, the pyrochlore and kagome lattices are intimately related. Indeed, applying a magnetic field along the [111] direction of the pyrochlore structure allows the freezing out of the apical spins, and establishes a connection with the two dimensional physical characteristics of the kagome lattice. Provided the field is not too large, a degeneracy persists within the kagome planes: the 2 in — 2 out ice rule transforms into the kagome ice rule, with 2 spins pointing into each triangle, and 1 out, or vice versa [1]. In this context, we report here a study of the effect of a [111] field on the ground state of Nd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>. In this pyrochlore magnet, classical spin ice physics is considerably modified by the existence of transverse terms in the Hamiltonian: spin ice signatures are transferred in the excitation spectrum, taking the form of a flat *spin ice* mode [2]. Correspondingly, we show here that above about 0.25 T, a flat dynamic *kagome ice* mode forms in the excitation spectrum, featuring a "dynamic kagome ice" state [3]. Mean-field calculations using the XYZ Hamiltonian [4,5] adapted for the Nd ion account qualitatively for our observations, although some discrepancies point to the existence of more complex processes. More generally, our study highlights the key role of transverse terms in the physics of pyrochlore magnets. We shall put this point into broader perspective, in the light of recent neutron scattering results obtained in other quantum spin ice candidates as for instance Pr<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> [6].

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#### Kinetic frustration induced supersolid in the S=1/2 kagome lattice antiferromagnet in a magnetic field.

X. Plat (RIKEN), T. Momoi (RIKEN), C. Hotta (Univ. of Tokyo)

We examine instabilities of the plateau phases in the spin-1/2 Heisenberg model in a magnetic field on the kagome lattice and find some emergent supersolid phases below the m=5/9 plateau. The wave functions of the plateau phases have a particular construction based on the building blocks of resonating hexagons and their surrounding sites. Magnon excitations on each of these blocks suffer from a kinetic frustration effect, namely, they cannot hop easily to the others because of cancellation between the various hopping paths. Therefore, the itineracy is thus weakened, and the system is driven toward the strong coupling regime, which together with the selected paths allowed in real space bears a supersolid phase. This mechanism is contrary to that usually proposed for the formation of supersolids (e.g. in lattice Bose gases), where the strong competing interactions suppress with each other, allowing a small kinetic energy scale to attain the itinerancy. Eventually, we find that the Kagome lattice host a supersolid state below m=5/9 in which the pattern of resonating hexagons are preserved from the plateau crystal state and only one-third of the originally polarized spins outside the hexagons dominantly join the superfluid component, *i.e.* participate in the magnetization process.

#### Topological protection of magnetic frustration.

#### Krishanu Roychowdhury

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We study the relationship between the physics to topology and frustration. Topological states of matter exhibit zero modes which are distinct from the ones arising from symmetry breaking. In other words, a zero mode must exist at the interface of two topologically distinct states across which the topological invariant differs. On the other hand, the existence of zero modes that are not symmetry related is a prominent aspect of frustrated systems as well. Taking cues from these two apparently different phenomena, we attempt to classify types of frustration using topology. We introduce an essential element in the formalism, namely the rigidity matrix, which is a non-Hermitian matrix and decides the topology of the zero modes in a frustrated magnet. Further developments of the theory rely on combining the recent developments in our understanding of Maxwell constraint counting [?] and generalizing the ten-fold way classification of Hermitian matrices to non-Hermitian matrices. The result is a three-fold way classification for each Maxwell counting index including both the isostatic and non-isostatic magnetic systems. We illustrate the classification by demonstrating the existence of a new vortex-like invariant for real rigidity matrices using random matrices and models of KHAF. Surprisingly in the latter, we discover topological properties of kagome coplanar states. So by classifying all the rigidity matrices, we answer the question of the origin of frustration in the form of accidental degeneracy in a wide class of frustrated magnets by linking it to topological invariants.

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#### $Dy_2ScNbO_7$ : a new spin ice candidate?

Megan Rutherford (UWinnipeg), C. Mauws(UofManitoba), S. Haravifard (Duke), C. Marjerrison (McMaster), G. Luke (McMaster), J. Beare (McMaster), D. Herbert (UofManitoba), J. Ritch (Uwinnipeg) and C. R. Wiebe (UWinnipeg) — Using standard solid state methods, Dy2ScNbO7, a member of a new series of pyrochlore oxides was synthesized. While the A-site is occupied by the magnetic Dy3+ cation, the B site is split into a mixture of disordered Sc3+ and Nb5+ cations. It appears that Dy2ScNbO7 has low temperature spin ice state that is similar to the titanate analogue, Dy2Ti2O7. Despite its similarities, Dy2ScNbO7 exhibits much faster spin dynamics than any other dysprosium spin ice candidate. Attempts to grow single crystals of Dy2ScNbO7 have been successful using the floating zone image furnace. Recent characterization results will be presented.

#### High-temperature ordered spin-ice structure in frustrated spinel CuCr<sub>2</sub>O<sub>4</sub>

K. Tomiyasu (Tohoku Univ.), S. Lee (KEK), H. Ishibashi (Osaka Pref. Univ.), Y. Takahashi (Tohoku Univ.), T. Kawamata (Tohoku Univ.), Y. Koike (Tohoku Univ.), T. Nojima (Tohoku Univ.), S. Torii (KEK), and T. Kamiyama (KEK)

We determined the magnetic structure in  $CuCr_2O_4$ , of which the research began 60 years ago [1,2], by a combination of time-of-flight high-resolution neutron diffraction and irreducible representation analysis. A new intermediate temperature phase is explicitly confirmed between 125 K and 155 K and is identified as emergence of a collinear magnetic long-range order in Cr pyrochlore lattice. Along with Shannon-Penc-Motome's theory [3], by replacing the collinear up/down by the ice in/out, this magnetic structure can be translated to the equivalent structure of ordered spin ice like in pyrochlore  $Tb_2Sn_2O_7$  [4,5], which has been experimentally unreported. Our finding would trigger the exploration and expansion of intriguing spin-ice physics, which have been restricted below a low temperature of  $\sim 1$  K in f-electron pyrochlores, in a readily accessible high-temperature range in other materials.

This study was financially supported by the MEXT and JSPS KAKENHI (JP17H06137, JP15H03692).

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#### Dynamical responses and instabilities of the Shastry-Sutherland model

Zhentao Wang (UTK), and Cristian D. Batista(UTK, ORNL)

The Shastry-Sutherland model is famous for holding an exact ground state solution for inter-dimer exchange J' < 0.7. In this exact ground state, each two spins on a dimer form an S=0 singlet. Single triplon excitations have a rather flat dispersion that renders perturbative treatments of the triplon-triplon interactions simply inadequate. In addition, the multiple competing length scales associated with the frustrated nature of this model also limits the applicability of numerical simulations on finite size clusters.

We introduce an unbiased variational method to study static and dynamic T=0 properties of the Shastry-Sutherland model in the thermodynamic limit, both as a function of inter-dimer exchange J' and magnetic field h. The variational basis is generated systematically by dressing up the 1- and 2-triplon excitations via a systematic inclusion of quantum fluctuations. The accuracy of this method is controlled by the number of iterations, which controls the size of the variational space. By solving the model in the thermodynamic limit, we can obtain dynamical responses (relevant to neutron, Raman and inelastic X-ray scattering) with high resolution in momentum space. Moreover, we can unbiasedly predict instabilities near the exact dimer phase, induced by single or multi-triplon condensation. We will discuss several competing orders (magnetic and nematic) next to the dimer phase and reveal the resulting phase diagram.

# Valence-Bond-Glass Ground State and Singlet Gap in the Spin-1/2 Square-Lattice Random $J_1$ - $J_2$ Heisenberg Antiferromagnet $Sr_2CuTe_{1-x}W_xO_6$ .

M. Watanabe(Tokyo Inst. of Tech., Japan), N. Kurita(Tokyo Inst. of Tech., Japan) and H. Tanaka(Tokyo Inst. of Tech., Japan) —

B-site ordered double perovskites  $Sr_2CuTeO_6$  and  $Sr_2CuWO_6$  are magnetically described as spin S=1/2 quasi-two-dimensional square-lattice Heisenberg antiferromagnet with the nearest-neighbor interaction  $(J_1)$  and next-nearest-neighbor interaction  $(J_2)$ . The dominant exchange interaction is  $J_1$  in  $Sr_2CuTeO_6$  [1], while  $J_2$  is dominant in  $Sr_2CuWO_6$  [2]. We present the low-temperature magnetic properties of the mixed system  $Sr_2CuTe_{1-x}W_xO_6$  with exchange bond randomness. Polycrystalline samples of  $Sr_2CuTe_{1-x}W_xO_6$  (x=0,0.1,0.2,0.3,0.4,0.5,1) were synthesized by a solid-state reaction. We performed magnetization and specific heat measurements systematically. For  $0.1 \le x \le 0.4$ , the low-temperature specific heat has a large component proportional to temperature T above 1.2 K, although for T 1 the low-temperature specific heat is approximately proportional to T 2. This T-linear specific heat is characteristic of the frustrated quantum magnet with exchange randomness [3,4]. We also found that, below 1.2 K, the T-linear component decreases rapidly with decreasing temperature toward zero, which is insensitive to magnetic field up to 9 T. This is suggestive of the presence of the singlet-singlet excitation decoupled from magnetic field. These results indicates that the ground state of  $Sr_2CuTe_{1-x}W_xO_6$  is the valence-bond-glass state with a singlet gap.

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#### Emergent SU(4) symmetry and quantum spin-orbital liquid in $\alpha$ -ZrCl<sub>3</sub>

M. G. Yamada (ISSP), M. Oshikawa (ISSP) and G. Jackeli (Univ. Stuttgart)

Quantum spin liquids have been sought mostly on geometrically frustrated lattices or in anisotropic systems with an exchange frustration. Another way to realize quantum spin liquids is to enhance the spin-space symmetry from the conventional SU(2) to SU(N) but realization of such an enhanced symmetry in magnetic materials remains challenging. Here we propose a magnetic material  $\alpha$ -ZrCl<sub>3</sub> as a new candidate for such SU(N) magnetism, where the SU(4) symmetry emerges in the strong spin-orbit coupling limit [1]. In  $d^1$  transition metal compounds with edge-sharing anion octahedra, the spin-orbit coupling gives rise to a strongly bond-dependent hopping between the j=3/2 quartets, which is apparently not SU(4)-symmetric. However, in the honeycomb structure, a gauge transformation maps the system to an SU(4)-symmetric Hubbard model. In the strong repulsion limit at quarter filling, the low-energy effective model

becomes the SU(4) Heisenberg model on the honeycomb lattice, which cannot have a trivial gapped ground state, and is expected to host a gapless spin-orbital liquid based on the previous numerical calculations [2].

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#### Unification of Pinch-Points and Half Moons in U(1) Spin Liquids

Han Yan (OIST), Rico Pohle (OIST) and Nic Shannon (OIST)

Pinch-points in the dynamical structure factor are the most significant hallmark of U(1) spin liquids. However, less attention has been paid to another distinctive feature: the "half-moons" observed in a range of different experiments and simulations [1-6]. Here we unify both signatures in a single gauge—theoretical framework, in the context of the Heisenberg model on a breathing Kagome lattice. We find that the half moons are nothing other than pinch-points in spin-spin correlation on a dispersive band, leading to their characteristic crescent—like form on a constant—energy cross section. Moreover, pinch—points and half moons come from the divergence—free and curl—free components of the same emergent magnetic field. This can be demonstrated very simply for the model in applied magnetic field, where the respective band dispersions are determined by semi—classical equations of motion. Finally, we argue that the physical picture is rather generic, by illustrating similar features in molecular dynamics simulations and surveying experimental realisations in Ca<sub>10</sub>Cr<sub>7</sub>O<sub>28</sub>, Tb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> and Nd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>.

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#### Itinerant fermions on a triangular lattice: unconventional magnetism and other ordered states.

M. Ye, A. Chubukov (University of Minnesota)

We consider a system of 2D fermions on a triangular lattice with well separated electron and hole pockets of similar sizes, centered at certain high-symmetry-points in the Brillouin zone. We first analyze Stoner-type magnetism. We show that the type of magnetic order in zero magnetic field depends on the interplay between intra- and inter-pocket interactions, and is either 120° "triangular" order (same as for localized spins), or a collinear order with antiferromagnetic spin arrangement on two-thirds of sites, and non-magnetic on the rest of sites. We show that in both cases a magnetic field gives rise to an expected canting of a spin configuration. In addition, it triggers a time-reversal symmetric bond order. We then consider the interplay between spin-density order and superconductivity and charge order, by analyzing the flow of the couplings within parquet renormalization group scheme. We show that magnetism wins when the pockets are not too small. For very small pockets, the system may develop either superconductivity or unconventional charge order.

### Band structure, magnetic, and optical properties of $In_2Ir_2O_7$ .

A. Yaresko (MPI FKF, Stuttgart), K. Rabinovich (MPI FKF, Stuttgart), A. Boris (MPI FKF, Stuttgart), B. Keimer (MPI FKF, Stuttgart), A. Krajewska (MPI FKF, Stuttgart), T. Takayama (MPI FKF, Stuttgart), H. Takagi (MPI FKF, Stuttgart) Recently, a new iridate compound  $In_2Ir_2O_7$  with the pyrochlore structure has been synthesized. Because of the smallness of In ionic radius IrO octahedra in this compound are more distorted than in other pyrochlore iridates and stronger mixing of  $j_{\rm eff}=1/2$  and  $j_{\rm eff}=3/2$  states can be expected. We calculated band structures and optical conductivity spectra of  $In_2Ir_2O_7$  and  $Y_2Ir_2O_7$  assuming all-in-all-out magnetic order and compared them to the experimental spectra obtained from ellipsometry measurements. Experimental temperature dependence of the optical conductivity is simulated by averaging spectra calculated for different magnetic configurations. By comparing their total energies we estimate the strength of Dzialoshinskii-Moriya interaction in these compounds.

### 0.23 Poster Session III

Friday 7/13

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1. R. R. Das (IIT Madras Chennai, India)
                2. S. Dengre (Technical University Dresden)
                          3. M. Enjalran (SCSU)
                          4. V. Favre LQM, EPFL
                            5. J. Fu (Minnesota)
         6. L. G'alisov'a (Technical University of Košice, Slovakia)
                 7. D. Gotfryd (IFT University of Warsaw)
                             8. D. Hirai (ISSP)
   9. N. B. Ivanov (ISSP-Bulgarian Academy of Sciences, Sofia, Bulgaria)
                           10. L. Jaubert (CNRS)
                 11. W. Jin (University of Waterloo, Canada)
                  12. K. Karl'ová (UPJS, Košice, Slovakia),
        13. S.-H. Lee (Department of Physics, University of Virginia)
                         14. Sangjin Lee (KAIST)
                     15. Yasin Maganda (MEMO UNIV)
                          16. S. Nakosai (RIKEN)
                        17. A. Otsuka (Kyoto Univ.)
                      18. Geet Rakala (OIST, Okinawa)
                     19. J. D. Reim (Tohoku University)
                          20. K. Remund (OIST)
                                21. L. Rossi
                     22. Antonio Ruotolo (HK CityU)
23. Alexandros Samartzis(Helmholtz-Zentrum, Technische Universität Berlin)
            24. L. Ø. Sandberg (University of Copenhagen, ESS)
                  25. C. Sarkis (Colorado State University)
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                          45. H.J. Yang (KAIST)
                        46. X.-P. Yao (Fudan Univ.)
                            47. X. Zhang (JHU)
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#### Multiple magnetic transitions, short range ferromagnetic correlation and Exchange bias in a layered perovskite.

R. R. Das (IIT Madras Chennai, India), A.K.Bera (BARC Mumbai, India) and P.N. Santhosh (IIT Madras Chennai, India).

Majority of the transition metal oxides such as monoxides (MO), perovskites  $(AMO_3)$  and Ruddlesden-Popper series  $(A_{2n-1}M_nO_{3n+1})$ ,[1] [ where A can be rare earth or alkaline earth ions or both and M are transition metal ions ] spinel compounds crystallize with M-O-M layers as well as MO symmetric (octahedral, tetrahedral etc) complexes crystal structure. Our aim of this work is to synthesis a novel material and study detail magnetic properties. Here we have focused on single layered perovskite of RP series. We have chosen Nd/Sr as rare-earth ion/alkaline earth ion and Mn and Co as transition metal ions to study the magnetic properties of this layered RP systems.

We have performed detail magnetic susceptibility and powder neutron diffraction measurements to study the magnetic properties of this compound. The magnetization measurement revealed multiple magnetic transitions along with signature of glassy behaviour with magnetic atoms orientated randomly in a crystal structure. These measurements evidenced three magnetic transitions at 175, 100 and 25 K respectively. The higher temperature is associated with the ferromagnetic transition which is weak in nature and the lower transition is corresponds to antiferromagnetic transition and 25 K corresponds to spin glass transition. But from neutron diffraction we confirmed competing magnetic interactions between Nd, Mn and Co leads to the frustration and absence of long range ordering in the present systems. We have also observed the presence of Griffith singularities in the paramagnetic regions which embedded in a ferromagnetic matrix. Because of competing magnetic interactions we have also observed a large exchange bias below 25 K.

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#### Frozen state and spin-gap behavior in a new kagome magnet Fe<sub>4</sub>Si<sub>2</sub>Sn<sub>7</sub>O<sub>16</sub>: An NMR study

S. Dengre (Technical University Dresden), R. Sarkar (Technical University Dresden), M.C. Allision (The University of Sydney), T. Söhnel (University of Auckland), C.D. Ling (The University of Sydney), J. Gardner (Neutron Group, Natl Synchrotron Rad Res Ctr), H.-H. Klauss (Technical University Dresden) Fe<sub>4</sub>Si<sub>2</sub>Sn<sub>7</sub>O<sub>16</sub> is a new Fe based kagome

system with a  $f=\theta/T_N\approx 3.6$ . The system consists of alternate stacking of kagome layer formed from edge sharing FeO<sub>6</sub> (S=2) and SnO<sub>6</sub> octahedra and stannate layer FeSn<sub>6</sub> (S=0). Fe<sub>4</sub>Si<sub>2</sub>Sn<sub>7</sub>O<sub>16</sub> is a classical homologue to a famous kagome compound herbertsmithite, a suitable candidate to realize quantum spin liquid phase.  $^{(117/119)}$ Sn nuclear magnetic resonance (NMR) allows us to selectively probe the static and dynamic magnetism of different Fe-layers. While the NMR shift vs bulk susceptibility plot follows linear relation down to 10 K confirming the absence of foreign phases in the vicinity of kagome plane, the considerable line broadening below 10 K indicates the distribution of static internal field. NMR spin-lattice/spin relaxation rate  $(1/T_1)/(1/T_2)$  reflect the slowing down of spin fluctuations at  $\sim 3$  K associated with the static magnetism of Fe-kagome layer. Additionally,  $(1/T_1)$  and  $(1/T_2)$  temperature dependency show a spin-gap behaviour with  $\Delta \sim 6.5$  K. [1]. 1. Ling *et al.* Phys. Rev. B 96, 180410(R)

#### Frustration driven metal insulator transition in 1/3-filled Hubbard model.

M. Enjalran (SCSU), R. Scalettar (UCD) —

The metal insulator transition (MIT) has been an active research topic in strongly correlated physics for decades.[1] With better materials and advances in theory and numerical methods, much has been learned about the nature of correlated phases near a MIT. It has been recognized that the strength of the electron-electron interactions and the filling fraction are important drivers of a MIT.[2] With the discovery of material systems where strong interactions coexist within a geometrically frustrated lattice environment, new phases of matter have been observed in experiments and corresponding theoretical explanations have been proposed.[3] Charge, magnetic, and orbital degrees of freedom can all be relevant in systems that undergo a MIT. The Hubbard model and its variants encapsulates the fundamental physics of material systems with this rich parameter space. The physical picture provided by the Hubbard model is further complicated when the lattice geometry is based on a triangular motif because electron hopping is geometrically frustrated. Focusing on charge and magnetic degrees of freedom only, we present results from mean field and quantum Monte Carlo calculations of the MIT in the 1/3 filled Hubbard model on the triangular lattice. In the mean field limit, the Hubbard model (*U* only) undergoes a two-step process where a paramagnetic metal develops noncollinear magnetic correlations

at a finite interaction strength,  $U^*/t \approx 4.70$ , followed by a MIT to a charge ordered and partially ordered magnetic state at  $U_c/t \approx 5.10$ . In the insulating phase, excess charge density and collinear antiferromagnetic (AFM) order define a honeycomb substructure of the parent triangular lattice. The remaining sites define a triangular substructure with reduced charge density and paramagnetism. In the absence of repulsive nearest neighbor Coulomb interactions (V), on-site interactions and frustrated hopping compete to select a state which relieves the frustration. Because the insulating phase breaks a discrete symmetry of the lattice, a finite temperature phase transition can be studied for  $U/t > U_c/t$ . We observe that the MIT occurs at  $T_c/t \approx 0.16$ , is weakly dependent on U, and is weakly first order. The constrained path quantum Monte Carlo (CPQMC) method is used to study the stability of the insulting state in the presence of quantum fluctuations.[4] Preliminary results from these calculations and an analysis of the performance of the CPQMC method will be presented.

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#### A Novel Kagome-like Cu<sub>2</sub>OSO<sub>4</sub> Crystal

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Low dimensional, geometrically frustrated antiferromagnets are at the forefront of condensed matter research. Materials with antiferromagnetic interactions between spins on a triangle lattice inherently exhibit large frustration between similar energy ground states giving rise to new behavior. Recently, experimental and theoretical results indicate that the kagome lattice can host spin liquid state[1]. The kagome lattice is an enticing example; however, various effects hinder its highly degenerate spin-liquid state and instead select a single magnetic ground state. It is therefore worthwhile to study nearly-kagomé compounds in an attempt to discern what precisely stops formation of the spin-liquid. We successfully synthesised a novel kagome like single crystal of Cu<sub>2</sub>OSO<sub>4</sub> and report here its magnetism, since it has strong antiferromagnetic interactions on a diamond-kagomé lattice. Very little was previously published and the only experiment performed were always done on powder samples[2]. We studied the magnetic excitation spectra of Cu<sub>2</sub>OSO<sub>4</sub> in order to help elucidate the mechanisms by which spin-liquid formation fails. We will present thermodynamic measurements, such as specific heat and magnetisation results, as well as neutron and X-ray diffraction data. We also recently measured large swaths of reciprocal lattice, energy space thanks to time of flight, inelastic neutron scattering. We will thus present the latest results analysed on this compound and their interpretation, in order to explain why the spin-liquid state fails to form in this compound and understand better criteria for spin liquid formation on the kagome

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Majorana representations of spin and an alternative solution of the Kitaev honeycomb model J. Fu (Minnesota), J. Knolle (Imperial College London) and N. B. Perkins(Minnesota) —

Based on the Dirac spinor representation of the SO(4) group, we discuss the relationship between three types of representation of spin in terms of Majorana fermions, namely the Kitaev representation, the SO(3) representation and the SO(4) chiral representation. Comparing the three types, we show that the Hilbert space of the SO(3) representation is different from the other two by requiring pairing of sites, but it has the advantage over the other two in that no unphysical states are involved. As an example of its application, we present a new alternative solution of the Kitaev honeycomb model. Our new solution involves no unphysical states which enables a systematic calculation of physical observables. Finally, we discuss an extension of the model to a more general exactly soluble  $Z_2$  gauge theory interacting with

complex fermions.

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# ADIABATIC TEMPERATURE CHANGES NEAR PHASE TRANSITIONS OF THE ISING DECORATED TRIANGULAR LATTICE.

L. Gálisová (Technical University of Košice, Slovakia)

We consider the mixed-spin Ising model on a decorated triangular lattice, where the spins at nodal lattice sites ( $\sigma = 1/2$ ) are coupled with three decorating spins (s = 3/2) through the ferromagnetic exchange interaction, and with remaining ones through the antiferromagnetic interaction. The system represents an extension of the spin-1/2 Fisher super-exchange model on a square lattice [1], which allows an exact examination of the magnetic-field effect in 2D. The presented numerical results follow our recent study on magnetic and magnetocaloric properties of the model [2]; they clarify the magnetocaloric effect (MCE) in its classical interpretation, namely as an adiabatic temperature change during the magnetic field variation. In particular, isentropic temperature changes as functions of the external magnetic field and temperature dependencies of the adiabatic temperature change are investigated in detail. It is demonstrated that the most pronounced temperature change during the adiabatic (de)magnetization process can be observed in a vicinity of the discontinuous field-induced phase transitions and also slightly above zero field if the entropy is set to be sufficiently close to the residual value found at the respective critical field. A rapid temperature drop up to the zero value detected in a proximity of the zero field points to a refrigeration potential of the model, which may be attractive for technological applications. At finite temperatures, the pronounced MCE can be observed near continuous temperature-induced phase transitions. The negative minima in temperature dependencies of the adiabatic temperature change clearly point to the inverse MCE in this region. It is confirmed that the relationship between the minimum adiabatic temperature change and the applied magnetic field is linear.

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#### Magnetic ordered moment for the extended Kitaev - Heisenberg model.

D. Gotfryd (IFT University of Warsaw), J. Rusnačko (CEITEC Masaryk University Brno), K. Wohlfeld (IFT University of Warsaw), G. Jackeli (MPI Solid State Research, Stuttgart), J. Chaloupka (CEITEC Masaryk University Brno), and A. M. Oleś (Jagiellonian University) —

We present the global phase diagram and the magnetic moment in phases with long-range order (Néel, ferromagnetic, zigzag, and stripy) — its size and direction — for the Kitaev–Heisenberg (KH) model [1] and for the extended KH model [2–4], obtained via linearized and self–consistent cluster mean field theory (CMFT). We evaluate quantum fluactuations in ordered phases and justify why the disordered Kitaev spin liquid phase has a much broader range of stability when the Kitaev interactions are ferromagnetic. Comparison with the results given by other methods (exact diagonalization, linear spin-wave theory) is also included [5].

This work is supported by NCN under Projects 2012/04/A/ST3/00331 and 2016/23/B/ST3/00839. [1] J. Chaloupka, G. Jackeli, G. Khaliullin, Phys. Rev. Lett. **105**, 027204 (2010); **110**, 097204 (2013); [2] J. G. Rau *et al.*, Phys. Rev. Lett. **112**, 077204 (2014); [3] J. G. Rau and H. Y. Kee, arXiv:1408.4811 (2014); [4] J. Chaloupka and G. Khaliullin, Phys. Rev. B **92**, 024413 (2015); **94**, 064435 (2016); [5] D. Gotfryd, J. Rusnačko, K. Wohlfeld *et al.*, Phys. Rev. B **95**, 024426 (2017)

# One-dimensionalization by frustration in the anisotropic triangular lattice of the 5d quantum antiferromagnets $A_3 \text{ReO}_5 \text{Cl}_2$ (A = Ca, Sr, and Ba).

D. Hirai (ISSP), K. Nawa (IMRAM), T. Yajima (ISSP), M. Kawamura (ISSP), T. Misawa (ISSP), and Z. Hiroi (ISSP) — The anisotropic triangular lattice (ATL) provides us with a unique playground for studying spin liquids existing between one and two dimensions. Anisotropy of the magnetic interaction on the triangular lattice is expected to lead to a variety of quantum phases including spiral order, gapless and gapped spin liquid phases [2]. However, the number of model compounds is limited. We report here new 5d quantum antiferromagnets A<sub>3</sub>ReO<sub>5</sub>Cl<sub>2</sub> (A = Ca, Sr, and Ba), where Re<sup>6+</sup> ions carrying Heisenberg spin-1/2 form an ATL. In spite of the substantial two-dimensionality, one-dimensionality is clearly observed in the magnetic susceptibility and heat capacity data: each of these compounds shows a broad peak in

the temperature dependences of magnetic susceptibility, which is nicely fitted by the Heisenberg spin-1/2 chain model, and a *T*-linear heat capacity with a consistent magnitude of the coefficient is observed at low temperatures. This reduction of dimensionality from ATL to decoupled spin chains must be caused by geometrical frustration. This family of compounds can be a good model system to study the Heisenberg spin-1/2 ATL in a systematic way.

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#### HEISENBERG SPIN CHAINS WITH THREE-BODY EXCHANGE INTERACTIONS

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The Heisenberg spin chains with two kinds of site spins  $(S_1,S_2)$  define realistic prototype models admitting extra isotropic three-body exchange terms which can drive the chain into exotic spin phases. In this work, based on density-matrix renormalization group and exact-diagonalization numerical calculations, we study the role of an external magnetic field on the recently established quantum phase diagrams for systems with  $(S_1, S_2) = (1, 1/2)$  and (3/2, 1/2) [1-3].

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#### Reentrance behaviour in the vicinity of classical spin liquids.

L. Jaubert (CNRS), O. Benton (RIKEN), K. Essafi (Paris), R. Pohle (OIST), M. Udagawa (Gakushuin), J. Oitmaa (UNSW), R. Singh (UC Davis), N. Shannon (OIST) —

Quantum critical points famously separate different phases at zero temperature via a continuous phase transition. Their effects are being felt over a broad temperature range, whose quantum critical fluctuations often support neighbouring exotic magnetic phases. In this poster, we will explore its classical analogue when one of the two neighbouring phases is a spin liquid. The enhancement of symmetry at this zero-temperature boundary would naively suggest a "more disordered" phase than the neighbouring spin liquid. However, this enhanced ground-state manifold may actually allow for critical fluctuations (soft modes) to concentrate on regions of the phase space that are otherwise inaccessible at low temperature. Order by disorder then plays its role, and the magnetic order of this high-symmetry point spreads like a fan at finite temperature. This fan gives rise to a reentrant behaviour above the spin liquid, and is continuously connected to more traditional order on the other side of the phase diagram. When order by disorder is not possible, then an extension of the idea of reentrance is possible for the competition between disordered spin liquids at finite temperature. To illustrate the different facets of this physics, several models will be discussed in two and three dimensions.

#### Spin-current order in antiferromagnetic zigzag ladder.

W. Jin (University of Waterloo, Canada) and O. Starykh (University of Utah, USA)

Here we study the stability of the collinear up-up-down phase in the 1/3 magnetization plateau in a zigzag ladder, which is a frustrated spin chain with competing nearest and next-nearest neighbor coupling  $J_1$  and  $J_2$ . The classically unfavorable 1/3 magnetization plateau survives through a large range away from the Majumdar-Ghosh point  $(J_2/J_1=1/2)$ . Via the semi-classical large-S expansion, we find that near the end of plateau, quantum fluctuations induce a two-magnon instability. This instability corresponds to a spin current (bond nematic) state as was proposed in Phys. Rev. Lett. 110, 217210 (2013) for a two-dimensional spatially anisotropic triangular lattice antiferromagnet. We find that the width of this bond nematic phase scales  $1/\sqrt{S}$ , which is much stronger than  $1/S^2$  dependence found on the triangular lattice.

We propose  $CaV_2O_4$  [1] and  $Cu_3V_2O_7(OH)_2 \cdot 2H_2O$  [2] as possible candidates to search for the experimental realization of spin nematic order in antiferromagnets. Unlike the ferromagnetic  $LiCuVO_4$  [3] chain-like candidate, which may host a similar bond-nematic state within a narrow magnetic field range around 40 T and just below saturation, in our model, this novel order appears at a magnetic field that is 1/3 of its saturation value, which is much lower than 40 T. The model

considered may underpin a more experimentally accessible alternative to study and observe the long sought spin nematic order.

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# Magnetization process and low-temperature thermodynamics of a mixed spin-1 and spin-1/2 Heisenberg chain. K. Karlová (UPJŠ, Košice, Slovakia), J. Strečka (UPJŠ, Košice, Slovakia)

The mixed spin-1 and spin-1/2 Heisenberg octahedral chain with regularly alternating monomeric and square-plaquette sites is studied within the framework of localized-magnon approach. It is shown that the model belongs to the class of flat-band systems with two dispersive and three dispersionless one-magnon energy bands, whereas one of the flat bands becomes lowest in energy in a highly frustrated parameter space. The low-temperature magnetization curve and thermodynamics of the mixed spin-1 and spin-1/2 Heisenberg octahedral chain is satisfactorily described by a two-component lattice-gas model taking into account the lowest-energy localized one- and two-magnon states. It is demonstrated that the low-temperature magnetization curve shows an abrupt magnetization jump at zero magnetic field towards the intermediate one-third plateau apart from another two magnetization jumps associated with presence of the intermediate two-thirds plateau. Moreover, it has been found that the field dependencies of the specific heat exhibit outstanding double-peak structure around each magnetization jump. The analytical results stemming from the localized-magnon approach were corroborated by the exact diagonalization method. In the rest of the parameter space we have accomplished DMRG calculations in order to construct the overall ground-state phase diagram, which involves a rich diversity of quantum phases including two quantum ferrimagnetic ground states, two spin-liquid ground states, Haldane phase, monomer-tetramer phase and magnon-crystal phase.

#### Memories of spin jam and spin glass.

S.-H. Lee (Department of Physics, University of Virginia) Author (shortAffil), Author(short Affil) and Author (short Affil) Aging and memory effects have been key features of glassy systems due to the intrinsic slow dynamics. The thermo-remanent magnetization (TRM) method is the most effective way so far to investigate these effects. Recently, we have performed the thermo-remanent magnetization (TRM) measurements on several magnetic glassy materials, including magnetic alloys, frustrated magnets, high temperature superconductor-related materials, and Kitaev-related spin-orbit Mott insulators.[1-2] Our TRM results show that scaling of magnetic memories with time can be used to classify magnetic glassy materials into two distinct classes, spin jam and spin glass. Most densely populated magnets exhibit similar memory behavior characterized by a relaxation exponent of  $1 - n \approx 0.6(1)$ . This exponent is different from  $1 - n \approx 1/3$  of dilute magnetic alloys that was ascribed to their hierarchical and fractal energy landscape, and is also different from 1 - n = 1 of the conventional Debye relaxation expected for a spin solid, a state with long range order. Furthermore, our systematic study on dilute magnetic alloys with varying magnetic concentration exhibits crossovers among the two glassy states and spin solid.[1,2]

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#### Spin-lattice Coupling in U(1) Quantum Spin Liquids

Sangjin Lee (KAIST), Leon Balents(KITP), and Eun-Gook Moon (KAIST)

Quantum spin liquids (QSLs) are exotic phases with intrinsic massive entanglements. Instead of microscopic spins, fractionalized particles and gauge fluctuations are emergent, which is revealing QSLs' exotic natures. In the pyrochlore

system with strong spin-orbit coupling, U(1) QSL phase are suggested to appear, which contain emergent photons, gapless excitations without breaking any symmetries, as well as electric and magnetic monopoles. Interplay between emergent degrees of freedom of QSLs and conventional degrees of freedom is one of the key issues in QSLs. In this presentation, we investigate this interplay by using spin-lattice couplings. In the U(1) QSLs, spin-lattice coupling is fundamentally different from one in magnetically ordered phases. We construct a general theory for spin-lattice coupling and characteristic interplay between phonons and emergent photons with a symmetry-argument. We show that emergent photons are qualitatively more stable than phonons at low temperature. We also propose mechanisms to detect emergent photons in experiments such as sound attenuation and thermal transport.

#### Organic diamond antiferromagnet: 3D Spin Liquid candidate.

A. Otsuka (Kyoto Univ.), M. Maesato (Kyoto Univ.), M. Tsuchiizu (Nara Women Univ.), A. Nakao (CROSS), H. Yamochi (Kyoto Univ.), T. Hiramatsu (Meijo Univ.), Y. Yoshida (Kyoto Univ.), G. Saito (Meijo Univ.) —
 Diamond lattice with a half-filling band provides a fascinating playground for frustrated spin liquids on the Mott insulating system and three-dimensional Dirac semimetals on the itinerant system. We present an rare example of organic diamond-lattice Mott insulator (ET)AG4(CN)5, one of the co-products of the quantum spin liquid κ-(ET)2Ag2(CN)3 [1]. Despite the antiferromagnetic exchange coupling of 220 K, the long-range magnetic order occurs at 100 K. By applying pressure, the transition temperature is enhanced up to 195 K and then suppressed toward the quantum critical point above 3 GPa. We also discuss the effects of spin-orbit coupling and inversion symmetry breaking that give rise to the Dzyaloshinskii-Moriya interaction.

[1] Y. Shimizu et al. Phys. Rev. Lett 117, 107203 (2016).

#### Magnetic monopole supercurrent through a quantum spin ice junction.

S. Nakosai (RIKEN), S. Onoda (RIKEN, RIKEN CEMS)

Quantum spin liquids are novel states of magnetic materials showing a long-range quantum entanglement and topological order. They are characterized by emergent gauge fields by spinons carrying fractionalized spin quanta which behaves as quantized sources and sinks of the magnetic field. When monopoles are condensed to form a long-range magnetic order, monopoles and gauge fields are confined and screened. However, we show that monopole supercurrent can flow across a junction of two ferromagnets that are weakly linked through and placed on top of the U(1) quantum spin liquid when a gauge-invariant phase difference of spinons across the junction is generated by, for example, quenching or an applied electric voltage parallel to the junction[1]. This phenomenon may provide a way to a new paradigm of dissipationless control of magnetism.

#### [1] **SN** and S. Onoda, arXiv 1801.03117

A. Otsuka (Kyoto Univ.), M. Maesato (Kyoto Univ.), M. Tsuchiizu (Nara Women Univ.), A. Nakao (CROSS), H. Yamochi (Kyoto Univ.), T. Hiramatsu (Meijo Univ.), Y. Yoshida (Kyoto Univ.), G. Saito (Meijo Univ.) —
 Diamond lattice with a half-filling band provides a fascinating playground for frustrated spin liquids on the Mott insulating system and three-dimensional Dirac semimetals on the itinerant system. We present an rare example of organic diamond-lattice Mott insulator (ET)AG4(CN)5, one of the co-products of the quantum spin liquid κ-(ET)2Ag2(CN)3 [1]. Despite the antiferromagnetic exchange coupling of 220 K, the long-range magnetic order occurs at 100 K. By applying pressure, the transition temperature is enhanced up to 195 K and then suppressed toward the quantum critical point above 3 GPa. We also discuss the effects of spin-orbit coupling and inversion symmetry breaking that give rise to the Dzyaloshinskii-Moriya interaction.

[1] Y. Shimizu et al. Phys. Rev. Lett 117, 107203 (2016).

#### $Z_6$ parafermions in the triangular lattice Ising antiferromagnet

Geet Rakala (OIST, Okinawa), Saumya Shivam (IITB, Mumbai) and Kedar Damle (TIFR, Mumbai)

Monte Carlo simulations using recently developed cluster algorithms for frustrated lattices have been used to study the phase diagram of a triangular lattice Ising antiferromagnet with ferromagnetic next-nearest and next-next-nearest interactions. In the presence of ferromagnetic next-nearest neighbour couplings, the spins form a three-sublattice ordered  $(\sqrt{3} \times \sqrt{3})$  state at low temperatures which melts via a two-step melting process. The intermediate power-law three-sublattice ordered phase is characterized by a temperature dependent exponent  $\eta(T) \in \left(\frac{1}{9}, \frac{1}{4}\right)$ . In this work, we study the nature of the melting transition as a function of increasing ferromagnetic next-next-nearest coupling strength. We find that the two-step melting pinches off, via a multicritical point  $\mathcal{M}_c$ , into a weak first order transition which separates the ferrimagnetic three-sublattice ordered state and a paramagnet. We numerically obtain estimates of the multicritical exponents at  $\mathcal{M}_c$  which are shown to match within errorbars with the values for the  $Z_6$  self-dual parafermionic conformal field theory constructed by Zamolodchikov and Fateev. We also demonstrate that the same exponents govern the behaviour of the corresponding pinch-off point of the power-law phase in the generalized six-state clock model studied by J. Cardy. Our results on the generalized clock model provide strong evidence in favour of a conjecture of Dorey et. al. identifying this pinch-off point with the  $Z_6$  parafermionic conformal field theory.

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# Neutron diffraction study and theoretical analysis of the antiferromagnetic order and diffuse scattering in the layered Kagome system CaBaCo<sub>2</sub>Fe<sub>2</sub>O<sub>7</sub>.

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The hexagonal swedenborgite,  $CaBaCo_2Fe_2O_7$ , is a chiral frustrated antiferromagnet, in which magnetic ions form alternating Kagome and triangular layers.[1] We observe a long range  $\sqrt{3} \times \sqrt{3}$  antiferromagnetic order setting in below  $T_N = 160\,\mathrm{K}$  by single crystal neutron diffraction.[2] Both magnetization and polarized neutron single crystal diffraction show that close to  $T_N$  spins lie predominantly in the ab-plane, while upon cooling the spin structure becomes increasingly canted due to Dzyaloshinskii-Moriya interactions.[3] The ordered structure can be described and refined within the magnetic space group P31m'. Diffuse scattering between the magnetic peaks reveals that the spin order is partial. Monte Carlo simulations based on a Heisenberg model with two nearest-neighbor exchange interactions [4,5] show a similar diffuse scattering and coexistence of the  $\sqrt{3} \times \sqrt{3}$  order with disorder. The coexistence can be explained by the freedom to vary spins without affecting the long range order, which gives rise to ground-state degeneracy. Polarization analysis [6] of the magnetic peaks indicates the presence of long-period cycloidal spin correlations resulting from the broken inversion symmetry of the lattice, in agreement with our symmetry analysis.

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#### **Equation of Motion for Spin-1 Magnets with Applications to Nematic Phases.**

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Frustrated magnetism is known to give rise to exotic and interesting phenomena, such as spin liquids or spin nematics. Obtaining a tool that would be able to describe the time evolution for both systems that do order conventionally and unconventionally, like a spin nematic, would therefore turn out to be very useful.

We develop a simple equation of motion for calculating the dynamics of spin-1 magnets. This method is based on a treatment of quantum spin-1 moments in the group U(3) and allows to treat both dipolar and quadrupolar moments on an equal basis. Thanks to the embedding into the algebra u(3), the equations of motion take a very simple form. By applying this method to the ordered phases of the spin-1 bilinear biquadratic model on a triangular lattice, we can make explicit comparison with already published flavour-wave theory results [1,2]. We show that the method can be applied to the 3-sublattice anti-ferromagnetic phase of the spin-1 bilinear biquadratic model on the triangular lattice and predict spin-1 and spin-2 excitations dispersion relations, which could be compared directly with experiments. Moreover, the equation of motion is easy to integrate numerically, thanks to its simple form, and could be applied to study the dynamics of spin liquids and topological defects in spin nematics.

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#### Negative thermal expansion in the high-field ferrimagnetic plateau state of a frustrated spinel.

L. Rossi, A. Bobel, J. Gerritsen, S. Wiedman, A. Khajetoorians and B. Bryant

Magnetic compounds with the spinel structure have been widely studied in the context of frustrated magnetism, since the pyrochlore sub-lattice can give rise to geometric frustration. Additionally, anomalous thermodynamic properties such as Negative Thermal Expansion (NTE) have been observed in some Cr based spinel compounds, such as  $CdCr_2S_4$  [?] and  $ZnCr_2Se_4$  [?]. NTE is thought to originate from the strong spin-lattice coupling and the competition between ferromagnetic and antiferromagnetic exchange.

The antiferromagnetic spinel CdCr<sub>2</sub>O<sub>4</sub> exhibits strong spin frustration, and as such remains paramagnetic down to 7.8 K. At this temperature there is a magnetostructural transition: the lattice distortion suppresses the spin frustration and allows a transition to a spin-spiral antiferromagnetic state. When a high magnetic field is applied to the antiferromagnetic state, a second phase transition occurs to a ferrimagnetic state which is characterized by a magnetization plateau with half of the saturation value. In this plateau the Cr tetrahedra show a three spin-up and one-down configuration [?, ?].

We performed low temperature capacitance dilatometry measurements on single crystal samples of CdCr<sub>2</sub>O<sub>4</sub> at high magnetic fields up to 30 T. Using this technique we were able to map the entire low-temperature phase diagram. Additionally, by measuring thermal expansion at static fields up to 30 T, we identified NTE in the ferrimagnetic plateau state. This novel observation gives a valuable insight into the nature of the spin-lattice coupling in the plateau state. We also aim to employ our unique high field Atomic Force Microscope to image the mesoscopic magnetic structure at the field transition to the plateau state.

#### Magnetically-induced transition from hopping to band conduction in Mn:ZnO thin films.

Antonio Ruotolo (HK CityU), Xiaolei Wong (HK CityU) and Qi Shao (HK CityU) — In europium (Eu) Gaudolinium (Gd) ternary alloys, the frustration between the ferromagnetically coupled Eu<sup>2+</sup> pairs in the antiferromagnetic Gd<sup>3+</sup> lattice leads to a giant negative megnetoresistance near their transition temperature [1]. The effect can be explained as magnetic activation of electrons localized on the Gd<sup>3+</sup> into the conduction band of the compound, where the activation energy is due to s-f exchange interaction. We here show that the same giant negative magnetoresistance can be induced in oxygen-deficient, manganese-substituted zinc-oxide (Mn-ZnO), in which p electrons from oxygen vacancies delocalized on Mn<sup>2+</sup> sites can be magnetically activated in the conduction band [2]. The study was carried out on films of Zn<sub>1-x</sub>Mn<sub>x</sub>O with x=0 (pure ZnO), 0.02, 0.04 and 0.08 grown by pulsed laser deposition on sapphire substrates. Oxygen vacancies ( $V_O$ 's) were introduced in the films by increasing the temperature of the substrate and decreasing the oxygen partial pressure during growth. A detailed characterization of our films

showed that all the Mn was in valence 2+, therefore Mn-O-Mn double-exchange interaction could be ruled out [3]. As the temperature was reduced, the resistivity of the films increased with distinct signatures of a transition from band- to hopping-conduction. A sharp decrease of resistance of the Mn-substituted films was measured when an external magnetic field was applied. The change of resistivity was found to increase with the concentration of Mn. Since ZnO is a transparent semiconductor, the magnetic activation of electrons to the band conduction could be probed by resorting to magneto-photoluminescence measurements. In fact,  $V_O$ 's are optically active defect centers that can form mono-centric or pair exciton complexes at low temperatures. Photoluminescence measurement at low temperature and applied magnetic field showed that  $V_O$ 's form deep-level F-centres, where electrons are localized. Electrons can hop between Mn- $V_O$  complexes under the application of an electric field. An applied magnetic field reactivates the electrons in the conduction band, resulting in a sharp drop of resistivity.

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### Spin dynamics of the ordered dipolar-octupolar pseudospin -1/2 pyrochlore Nd<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub>.

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The rare earth pyrochlore magnets have been extensively studied during the last decades due to their quintessential lattice for frustration which leads to exotic ground states with strong anisotropy (1). From this lattice the competition of crystal field, super-exchange and dipolar interactions can result in novel states, such as spin liquid, spin ice etc. The Nd3+ ion, on such a lattice has a Kramers doublet ground state with a dipolar-octupolar wavefunction leading to a fascinating phase diagram (2). Here we report first results of inelastic and polarized neutron scattering, on a new Nd-based pyrochlore, Nd2Hf2O7. Recent macroscopic measurements have revealed an ordered all-in all-out antiferromagnetic ground state with slow spin dynamics and a strongly reduced magnetic moment due to local fluctuations (3). Motivated by these interesting results, we performed low energy Inelastic Neutron scattering on a large single crystal grown by the floating zone technique. The results reveal long range magnetic order below T<sub>N</sub>=600mK. The excitations form a gapped flat band at energy DE 0.1meV reflecting the pinch-point pattern of a Coulombic phase. Above the flat band, collective dispersive excitations emerge from the pinch points. Linear spin-wave theory was used to determine the exchange parameters (Ja) applied in an appropriate Hamiltonian (4).

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#### Quantum fluctuations on a hyperkagome lattice

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Quantum spin liquid (QSL) states are exotic states of matter that feature strong quantum fluctuations leading to a disordered ground state at zero temperature with emergent quasiparticles that exhibit fractionalised excitations. The search for QSL states has been heavily focussed on lattices comprised of 2 dimensional (2D) corner sharing triangular structures of which the kagome system is most common. It is widely considered that equivalent 3 dimensional (3D) compounds would also display novel ground states. The pyrochlore and spinel structures that display a network of corner-sharing tetrahedra have been most heavily studied. In contrast, experimental examples of geometric frustration on a 3D networks of corner sharing lattices are less common, yet are theoretically considered to be highly promising for exotic states. A prominent, and only, example of a 3D cornersharing QSL is the hyperkagome compound Na<sub>4</sub>Ir<sub>3</sub>O<sub>8</sub>, which is a candidate for QSL ground states based on the 3d transition metal oxides, [1,2].

A second example for a 3D QSL is the rare earth based hyperkagome system Yb3Ga5O12 (YbGG). The Yb ions in YbGG realise a lattice of two interpenetrating hyperkagome structures. Spin-orbit coupled Yb<sup>3+</sup> ions sit in a local

environment with a coordination number of z = 4, similar to the local environment of the magnetic ions on a 2D kagome lattice. The specific heat indicates that the ground state is a Kramers doublet, separated from the excited doublet which can be found at 546 cm<sup>-1</sup> [3] thus providing a pseudo quantum spin, S = 1/2.

Magnetisation measurements determine a Curie-Weiss temperature  $\theta_{CW} = -118$  K with no indication of long range order down to  $T_N = 54$  mK [4] which gives YbGG an unusually high frustration index of  $\theta_{CW}/T_N \sim 2100$ . Specific heat measurements determined the development of short range magnetic correlations below 0.5 K and a lambda-transition at 54 mK while 170-Yb Mössbauer spectroscopy, determined no static magnetic order at temperatures below the lambda-transition. Indeed the specific heat measurements indicate that only 20% of entropy is frozen at the lambda point thus leaving the true ground state an open question [4,5]. It has recently been possible to synthesise YbGG and grow a single crystal suitable for neutron scattering studies. Recent neutron scattering results confirm the short range nature of the spin-spin correlations with unusual diffuse scattering features in both the elastic and inelastic channels. The implication for a QSL state in YbGG will be discussed.

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#### Partial Magnetic Order in Fe<sub>3</sub>PO<sub>4</sub>O<sub>3</sub>

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The magnetic frustration brought about by triangular motifs and competing antiferromagnetic interactions in Fe<sub>3</sub>PO<sub>4</sub>O<sub>3</sub> (spacegroup R3m) have been shown to lead to an unusual magnetic state below  $T_N = 163$  K. Below  $T_N$ , antiferromagnetic order is restricted to nanosized needle-like domains oriented along the c-axis, with the correlation length restricted to  $\xi = 7nm$  in the ab plane. Here we present single crystal neutron diffraction results, which reveal that this state does not select a preferred ordering wavevector in the ab plane, resulting in continuous rings of scattering rather than well-defined satellite Bragg peaks. The lack of a preferred incommensurate ordering wavevector can be understood in terms of the competition between  $J_1$  (nearest neighbor) and  $J_2$  (next nearest neighbor) interactions in a Heisenberg model, which produces a quasidegenerate manifold of ordering wavevectors. The inability to form long range coherent structure remains unexplained, however the restriction to small domain sizes in the ab plane implies the presence of a high density of topological defects. Determining the nature of these defects and the mechanism of their formation is an avenue for further research.

#### Quantitative signature of a continuous phase transition in artificial square ice.

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In recent years, artificial spin systems, consisting of elongated single-domain ferromagnetic nanomagnets placed on the nodes of two-dimensional lattices and coupled via their dipolar magnetic fields, have been used to address open questions in frustrated magnetism. However, the imaging techniques so far used, are severely constrained in time and spatial resolution. We have therefore recently developed x-ray resonant scattering to probe the magnetic configuration in artificial spin systems, which allows us to go beyond these limits in time and spatial resolution, and provide a means to determine, for example, the predicted phase transitions in artificial spin systems. As a result, we have been able to determine separately the contribution to the total magnetization of the nanomagnets belonging to each one of the two sublattices of artificial square ice [1] and to measured magnetic correlations in a highly dynamic artificial kagome spin ice with sub-70 nm Permalloy nanomagnets [2].

In this contribution, I will illustrate our recent results that establish the critical properties of the antiferromagnetic phase

transition in artificial square ice composed of superparamagnetic nanoelements with fluctuating magnetic moments, showing that it belongs to the two-dimensional Ising universality class [3]. Our work extends the applicability of such concepts from atomistic systems to mesoscopic magnets. We characterize the transition to the low temperature long-range-ordered phase expected for artificial square ice both experimentally and theoretically, combining soft x-ray resonant magnetic scattering experiments and Monte Carlo simulations. In addition, taking advantage of the flexibility in the design of the magnetic properties of our system, we have determined the influence of the proximity of the blocking temperature relative to the phase transition temperature, resulting in a dramatic change on the out-of-equilibrium dynamics due to critical slowing down at the phase transition.

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#### 120° Compass Model with Strong Quantum Fluctuations in $NaNi_2BiO_6$

Allen Scheie (Johns Hopkins University), Kate Ross (Colorado State University, CIFAR) Elizabeth Seibel (Princeton University), Jose A. Rodriguez-Rivera (NIST), Joel Tang (Johns Hopkins University), Robert Cava (Princeton University), and Collin Broholm (Johns Hopkins University).

We report the magnetic structure of honeycomb compound  $\mathrm{NaNi_2BiO_6}$ , which appears to host bond-dependent  $120^\circ$  compass model interactions. This compound orders along the c axis below  $T_{c1} = 6.3$  K and then in the plane below  $T_{c2} = 4.8$  K with the incommensurate ordering wave vector  $q = (1/3, 1/3, 0.154 \pm 0.011)$ . Magnetic entropy and neutron scattering both show that a significant fraction of the magnetic moment remains fluctuating at low temperatures, suggesting an unconventional partially-ordered magnetic phase. The in-plane magnetic correlations and superexchange pathways are consistent with a bond-dependent  $120^\circ$  compass model exchange—a cousin of the celebrated Kitaev exchange—which may be responsible for the observed magnetic structure.

#### Phase diagram of dipolar-coupled XY moments on disordered square lattices.

D. Schildknecht (ETH Zurich-Paul Scherrer Institute, CH), L. Heyderman (ETH Zurich-Paul Scherrer Institute, CH) and P. Derlet (Paul Scherrer Institute, CH)

The anisotropic dipolar interaction can lead to novel collective magnetic phenomena driven by frustration. In particular, through this anisotropy, the symmetry of a dipolar magnetic Hamiltonian is set by the point symmetry group of the underlying spatial lattice. For the two dimensional square lattice with continuous in-plane magnetic degrees of freedom, this fact leads to a continuously degenerate ground state, even though the Hamiltonian only supports a finite group. For the clean system, a perturbative spin wave analysis demonstrates that temperature selects the so-called striped phase from ground state manifold. In the present work we investigate the effect of dilution and positional disorder, constructing the full phase diagram via the parallel tempering Monte Carlo algorithm in terms of new order parameters, which are able to distinguish the different types of long-range order within the degenerate ground-state manifold. We find that for a finite temperature interval and disorder strength, dilution and positional disorder have a similar effect. Both select a long range order characterized by an arrangement of micro-vortex magnetic structures. We will show how this can be understood intuitively in terms of local flux closure.

#### Noncollinear magnetic ordering in a frustrated magnet: Metallic regime and the role of frustration.

Munir Shahzad (NTU, Singapore), Pinaki Sengupta (NTU, Singapore.)

We explore the magnetic phases in a Kondo lattice model on the geometrically frustrated Shastry-Sutherland lattice at metallic electron densities, searching for noncollinear and noncoplanar spin textures. Motivated by experimental observations in many rare-earth-based frustrated metallic magnets, we treat the local moments as classical spins and set the coupling between the itinerant electrons and local moments as the largest energy scale in the problem. Our results show that a noncollinear flux state is stabilized over an extended range of Hamiltonian parameters. These spin states can be quenched efficiently by external fields like temperature and magnetic field as well as by varying the degree of frustration in the electronic itinerancy and exchange coupling between local moments. Interestingly, unlike insulating electron densities that we discussed in paper I of this sequence, a Dzyaloshinskii-Moriya interaction between the local moments is not essential for the emergence of their noncollinear ordering.

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#### Ripple state in the $J_1$ - $J_2$ classical honeycomb-lattice Heisenberg antiferromagnet

T. Shimokawa (OIST, Japan) and H. Kawamura(Osaka Univ., Japan)

The  $J_1$ - $J_2$  classical honeycomb-lattice Heisenberg antiferromagnet is known as one of characteristic frustrated systems having infinitely degenerate ground states. Much attention has been paid especially to the thermal and quantum fluctuation effects due to the infinite degeneracy. The interest has been further enhanced recently because of an experimental observation of the spin-liquid state in S=3/2 honeycomb-lattice Heisenberg AF  $\mathrm{Bi}_3\mathrm{Mn}_4\mathrm{O}_{12}(\mathrm{NO}_3)$ , accompanied with a field-induced antiferromagnetism. [1]

Okumura  $et\ al\ [2]$  have investigated the  $J_1$ - $J_2$  classical honeycomb-lattice Heisenberg antiferromagnet with the aim of understanding the magnetic properties of  ${\rm Bi_3Mn_4O_{12}(NO_3)}$ . For  $1/6 < J_2/J_1 < 0.5$ , the ground-state manifold was known to form a closed "ring-like" curve in the wave vector space around the antiferromagnetic (AF) point. [3] They have found the emergence of the two exotic spin-liquid states accompanied with an field-induced antiferromagnetism; one is the "ring-liquid" state having a ring-pattern surrounding the AF point, and the other is the "pancake-liquid" state where the center of the ring is buried leading to the pancake-like structure. The ring degeneracy in the ground state could be a source of these exotic spin-liquid states.

In the previous study by Okumura  $et\ al$  in zero magnetic field, only a single-q spiral state has been found. From a theoretical view point, however, exotic multiple-q states are expected to be realized for the  $J_1$ - $J_2$  classical honeycomb-lattice Heisenberg system under fields, such as the triple-q skyrmion-lattice state realized in the classical triangular-lattice Heisenberg system.[4] Actually, we succeeded in finding several exotic multiple-q states in the  $J_1$ - $J_2$  classical honeycomb-lattice Heisenberg antiferromagnet under magnetic fields [5][6].

More recently, we newly find a more intriguing multiple-q state keeping the ring-like closed-curve intensity around the AF point in the spin structure factor as that in the "ring-liquid" state. The corresponding real-space spin configuration seems to be like a "water ripple", so that we call this state a "ripple" state [7]. In our presentation, we will talk about the detail of our finding for the ripple state and also discuss the relationship to the experimental measurements on  ${\rm Bi_3Mn_4O_{12}(NO_3)}$ .

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#### Discovery of new magnetic orders on pyrochlore spinels

GiBaik Sim(KAIST) and SungBin Lee(KAIST) —

Frustration in spin system can give rise to unique ordered states and as a consequence several physical phenomena are expected such as multiferroics, high temperature superconductors and anomalous hall effect. Here we report the "new magnetic orders" induced by anisotropic spin exchanges on pyrochlore spinels as the interplay of spin orbit coupling and geometrical frustration. Due to complicated superexchange paths of B-site spinels, we claim that anisotropic interaction between next-nearest neighbors play an important role. Based on the systematic studies of generic spin model, we argue that several classical spin states can be explored in spinel systems; local XY state, all-in all-out state, Palmer-Chalker state and coplanar spiral state. In addition, we reveal new types of magnetic phases with finite ordering wavevectors, labeled as 'octagonal (prism)' state and '(distorted) cubic' states. When the 'octagonal prism' state is stabilized, non-zero scalar spin chirality induces alternating net current in addition to finite orbital current and orbital magnetization even in Mott insulators. Finally, we also discuss the relevance of 'distorted cubic' state to the magnetic order of spinel compound GeCo<sub>2</sub>O<sub>4</sub>.

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#### Unconventional order-disorder phase transition in improper ferroelectric hexagonal manganites.

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The improper ferroelectricity in YMnO<sub>3</sub> and other related multiferroic hexagonal manganites are known to cause topologically protected ferroelectric domains that give rise to rich and diverse physical phenomena (Griffin *et al.*, 2012; Meier *et al.*, 2015). The local structure and structural coherence across the ferroelectric transition, however, are not well understood (Lilienblum *et al.*, 2015). Here we reveal the evolution of the local structure in YMnO<sub>3</sub> using a combination of neutron total scattering and first-principles calculations (Skjærvø *et al.*, 2017). The results show that, at room temperature, the local and average structures are consistent with the established ferroelectric ground state structure. On heating, both local and average structural analyses show striking anomalies consistent with increasing fluctuations of the order parameter angle from ~800 K up to the Curie temperature. These fluctuations result in an unusual local symmetry lowering into a continuum of structures on heating which coincides well with reported temperatures for which the observable polarization vanishes. This local symmetry breaking persists into the high-symmetry non-polar phase, constituting an unconventional type of order-disorder transition.

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# Effects of magnetisation patterns and emergent monopoles on the electronic structure of spin ice $Dy_2Ti_2O_7$ in photoabsorption measurements.

A. Szabó (Cambridge), C. Castelnovo (Cambridge) —

Spin ice, a frustrated magnetic system, exhibits several unusual features, including a highly degenerate (spin liquid) ground state and emergent magnetic monopole excitations. While experimental signatures of these properties have been observed in magnetisation and neutron scattering measurements, their effect on the electronic structure has not been explored. In this project, a simplified model for the electronic structure of spin ice Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> was developed to investigate the effects of the magnetic pattern of the localised Dy *f*-moments on the (insulating) band structure of the Ti *d*-electrons. Whereas a number of effects are potentially at play, including Aharonov–Bohm and Berry phases, we find that most of them have a largely negligible effect, with the exception of scattering due to the induced electric dipole moment on tetrahedra that host monopoles. This results in a perturbation of the band structure that is linear in the density of monopoles and may be observable in an experimentally measurable change in the tail of the photoabsorption spectrum.

# Quantized magnetization plateaus of a frustrated spin-1/2 Ising-Heisenberg model on triangulated Husimi lattice.

J. Strečka (UPJŠ) and C. Ekiz (AMU)

The geometrically frustrated spin-1/2 Ising-Heisenberg model on triangulated Husimi lattice is exactly solved in a magnetic field by combining the generalized star-triangle transformation with the method of exact recursion relations. The star-triangle transformation maps the investigated spin system onto the spin-1/2 Ising model on a Husimi lattice with the effective pair and triplet interactions, which is subsequently rigorously treated by making use of exact recursion relations. The ground-state phase diagram is rigorously calculated along with both sublattice magnetizations of the Ising and Heisenberg spins. It is evidenced that the total magnetization of the spin-1/2 Ising-Heisenberg model on triangulated Husimi lattice displays outstanding dependence on a magnetic field, which includes several intermediate magnetization plateaus of quantum origin at moderate values of the magnetic field. It is demonstrated that emergent quantized magnetization plateaus have either character of dimerized or trimerized ground states, which are in accordance with the reported ground-state phase diagram.

# Ising versus Potts criticality in low-temperature magneto-thermodynamics of a frustrated spin-1/2 Heisenberg triangular bilayer.

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Low-temperature magnetization curves and thermodynamics of a frustrated spin-1/2 Heisenberg triangular bilayer with the antiferromagnetic intra-dimer interaction and either ferromagnetic or antiferromagnetic inter-dimer interaction are investigated in a highly frustrated parameter region, where localized many-magnon eigenstates provide the most dominant contribution to a magneto-thermodynamics. Low-energy states of the highly frustrated spin-1/2 Heisenberg triangular bilayer can be accordingly found from a mapping correspondence with the effective spin-1/2 Ising model on a triangular lattice. The description based on the effective Ising model implies that the spin-1/2 Heisenberg triangular bilayer with the ferromagnetic inter-dimer coupling displays in a zero-temperature magnetization curve discontinuous magnetization jump, which is reduced upon increasing of temperature until a continuous field-driven phase transition from the Ising universality class is reached at a certain critical temperature. The spin-1/2 Heisenberg triangular bilayer with the antiferromagnetic inter-dimer coupling contrarily exhibits multistep magnetization curve with intermediate plateaus at one-third and two-thirds of the saturation magnetization, whereas discontinuous magnetization jumps observable at zero temperature change to continuous field-driven phase transitions from the universality class of three-state Potts model at sufficiently low temperatures. The results obtained from Monte Carlo simulations of the effective Ising model are confronted with full exact diagonalization data for the Heisenberg triangular bilayer in order to corroborate these findings.

#### Dynamical properties of $\alpha$ -RuCl<sub>3</sub> in magnetic fields

T. Suzuki and S. Suga (Univ. of Hyogo)

Honeycomb-lattice magnet  $\alpha$ -RuCl $_3$  has been received much attention, because this material is considered as one candidate material in the proximity of the Kitaev spin liquid (KSL) [1]. Although this material undergoes a phase transition to the zigzag ordered state at the Néel temperature  $T_{\rm N}\approx 7~{\rm K}$  [2,3], recent inelastic neutron-scattering (INS) measurements on this material have unveiled characteristic dynamical properties [3,4] possibly connecting to the spin excitation continuum in the Kitaev limit: The intensity at the  $\Gamma$  point survives beyond  $T\approx 100~{\rm K}$  that is quite far above  $T_{\rm N}$ . It has been pointed out that vicinity to the KSL is observable as the two-peak structure in the temperature dependence of the heat capacity C(T), even when the magnetic order is stabilized at a low temperature [5]. The heat capacity measurements on this material [4,6] have also shown the proximity of the KSL. It has been observed that there is a two-peak structure in C(T) and the higher temperature peak appears approximately at  $T\approx 100~{\rm K}$  [4]. Effective models for  $\alpha$ -RuCl $_3$  have been proposed so far and some of them successfully explain experimentally observed thermodynamic quantities and/or low-lying excitations. However they show qualitatively different features with each other and thus, the proper model of  $\alpha$ -RuCl $_3$  is still controversial.

In this study, we calculate dynamical spin structure factors of three *ab-initio* models [7-9] and an *ab-initio*-guided model [10] for  $\alpha$ -RuCl<sub>3</sub> by using an exact numerical diagonalization method. We also calculate temperature dependences of the heat capacity, the nearest-neighbor spin-spin correlation function, and the static structure factor by employing typicality approach [11,12]. The obtained results indicate that the four models fail in explaining both the INS experiments and the heat capacity measurements. In these four models, C(T) shows a prominent peak in the higher temperature region with

decreasing temperature. However, it is found that the peak temperatures in C(T) are too low in comparison with the observed values in the experiments. Thus, we propose an effective model with the strong ferromagnetic Kitaev coupling that is able to reproduce the above experimental features. To discuss further adequacy of the proposed model, we calculate the field dependence of the polarized teraheltz spectra. We find that the proposed model successfully reproduces the experimental results: the spin-gapped mode surviving up to an onset field where the magnetic order disappears and the almost liner response in the high field region. From the obtained numerical results, we argue that the feature of the low-energy magnetic excitation in  $\alpha$ -RuCl $_3$  is mainly characterized by the other interactions rather than the most dominant Kitaev interactions, such as the off-diagonal interactions on the nearest-neighbor pairs.

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### Magnetic Frustration in the Triangulated Kagome Lattice Cu9X2(cpa)6.

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The discovery of novel magnetism [1] in the 2-D layered compounds Cu9X2(cpa)6 (X = F, Cl, Br; cpa = anion of 2-carboxypentonicacid), abbreviated as CPA, led to additional data [2] and theoretical studies [3-5] that conjecture the ground state of this Heisenberg lattice is enigmatic and highly frustrated. The 2-D CPA framework has been described as a triangles-in-triangles (TIT) Kagome lattice or a triangulated-Kagome-lattice (TKL). As a metal organic framework (MOF) based on S = 1/2 copper(II) ions, the triangulated framework serves as a candidate material for studies on quantum spin liquids (QSLs). Spin interaction nets suggest that if the framework can be chemically manipulated, rich phase diagrams of topologically induced spin-liquid states should be produced, depending on the presence or absence of a ground state gap that could be deliberately engineered either chemically or through external pressure.[6] Since the key to expanding the utility of CPA lies in expanding the number of members in its material class, we recently reported CPA offers at least two strategies for chemical tunability.[7] We will discuss new synthetic results for additional material variability, as well as low temperature magnetic susceptibility, magnetization and heat capacity data that further demonstrate CPA can be chemically manipulated to controllably affect its low temperature physics. The new data confirm that signature features of TKL magnetism persist, specifically: i) large negative Weiss constant; ii) absence of zero-field phase transition down to 50mK; iii) temperature dependent minimum in XMT; iv) low temperature XMT values that are increasingly divergent at low fields; v) field dependence of magnetization at low temperatures suggestive of intermediate plateaus, and vi) heat capacity studies that demonstrate a field-induced phase transition can be obtained that, by extrapolation, approaches 0K in zero-field. These data produce a T-H phase diagram similar to Herbertsmithite [8,9] suggesting CPA is a viable candidate for further QSL studies. Supported by NASA via grant

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#### When Three is a Crowd: Entanglement of Quantum Spins on Tripartite Lattices.

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There are a number of interesting materials, which are built up of strongly coupled triangular plaquettes that form a breathing lattice. One example is the quantum spin liquid  $Ca_{10}Cr_7O_{28}$  which has been observed experimentally to suppress magnetic order down to 19mK, despite its predominantly ferromagnetic exchange interactions. This particular material has now been studied using classical monte-carlo methods, but a question that arises is whether there are fundamentally quantum excitations and how they arise.

In our work we approach a simpler version of this problem, namely the breathing monolayer kagome, by investigating the effects of local entanglement. We start by diagonalizing the Hamiltonian of a single triangle of interacting spins exactly. The full wavefunction of the lattice can then be expanded as a combination of all possible trimer eigenstates. Then we decompose the system into a multiboson basis of excitations on top of an ordered ground state [1]. We show that this reproduces results of linear spin-wave theory on the same lattice, whilst at the same time including the dispersion of higher spin excitations.

Whereas the effects of entangled excitations are normally not accounted for in spin-wave theory, multiboson theory gives a natural way to explore them at a local level in a basis that may be expanded by inclusion of more spins. As has been seen before this can serve to explain unconventional magnetic excitations in frustrated magnetism [2]. Having seen that this method works for the simple cases we can now apply it to more interesting geometries.

It is as if we are exploring the social life of an infinite number of spins by viewing them not as individuals, but as groups of three who are regarded as a clique by the rest of the lattice. That is when their quantum nature emerges, because in physics three's a crowd.

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### Emergent ferroelectricity in the S=1 kagomé magnet $Na_2Ti_3Cl_8$

Z.A. Kelly (Johns Hopkins University), T.T. Tran (Johns Hopkins University), T.M. McQueen (Johns Hopkins University) Kagomé lattice magnets have emerged as a versatile platform on which to discover and explore the underlying physics of quantum spin liquids and related states of matter, though experimental examples of ideal kagomé lattices remain rare. Interest has been growing in integer spin antiferromagnetic kagomé systems in search of various quantum ground states, such as the 2D valence bond solid. This ground state has a spin gap formed by entangled S=1/2 edge spins from termination of the S=1 kagomé lattice, a 2D analog to the Haldane state in S=1 chains. The S=1 kagomé lattice has also been theorized to host other exotic ground states such as the hexagonal singlet state as well as structural instabilities leading to spontaneous trimerization. Here we report the realization of an ideal S=1 kagomé in Na<sub>2</sub>Ti<sub>3</sub>Cl<sub>8</sub>. This material undergoes a discrete two-step trimerization on cooling, transforming from a centrosymmetric high temperature (HT)  $R\bar{3}m$  phase to non-centrosymmetric, ferroelectric intermediate (IT) and low temperature (LT)  $R\bar{3}m$  phases via successive first order phase transitions and the formation of metal-metal bonds. Symmetry mode decomposition analysis reveals the activation of the proper ferroelectric order parameter  $\Gamma_2^-$  upon trimerization. Thus Na<sub>2</sub>Ti<sub>3</sub>Cl<sub>8</sub> demonstrates a novel mechanism to obtain proper ferroelectricity driven by frustrated magnetism and metal-metal bonding, and highlights the rich physics arising from kagomé lattice materials.

# Randomness-induced ordering behavior of the frustrated $s=1/2\ J_1$ - $J_2$ Heisenberg model on the square-lattice with ferromagnetic and antiferromagnetic $J_1$

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In quantum spin systems, the quantum spin liquid (QSL) state has long received much attention as a novel state of matter. It was recently reported that the quenched randomness often plays an important role in stabilizing the QSL state in frustrated spin systems. [1-3] Such randomness-induced QSL state, called the random-singlet (RS) state, is observed in many frustrated lattice models so that the RS state might be realized in a wide class of frustrated quantum magnets with a certain amount of randomness without fine-tuning the details of interactions. In the present study, to get further insight into the universal character of the RS state, we study the random s = 1/2 quantum Heisenberg model on the square lattice, with the competing nearest- and the next-nearest-neighbor interactions  $J_1$  and  $J_2$ , by means of an exact diagonalization method. While we fix  $J_2$  to be antiferromagnetic, we treat not only the antiferromagnetic  $J_1$  but also the ferromagnetic  $J_1$ , to exami ne whether the RS state is ever possible in the ferromagnetic case. Randomness is introduced

by uniformly distributing the strength of  $J_1$  and  $J_2$  with the width  $\Delta$ , *i.e.*, uniformly distributed between  $[(1-\Delta)J_1,(1+\Delta)J_1]$  and  $[(1-\Delta)J_2,(1+\Delta)J_2]$ . In this model, the extents of both randomness and frustration can be varied by tuning the randomness parameter  $\Delta$  and the frustration parameter  $J_2$ , as in the case of the honeycomb  $J_1$ - $J_2$  model studied in [3]. For the square lattice, the number of nearest-neighbors is four, more than that on the honeycomb lattice, three, so that the magnetically ordered states is expected to be more robust against fluctuations compared to the honeycomb-lattice case. We get a ground-state phase diagram of the model in the randomness ( $\Delta$ ) versus the frustration  $(J_2/J_1)$  plane for both cases of ferromagnetic and antiferromagnetic  $J_1$ . We have found that not only the RS state but also the SG state is stabilized for stronger randomness depending on the  $J_2/J_1$ -value in the case of antiferromagnetic  $J_1$ , while only the SG state is stabilized in the case of ferromagnetic  $J_1$ . This observation suggests that the antiferromagnetic character of the main interaction is necessary to stabilize the RS state. For the antiferromagnetic  $J_1$ , the SG state is realized in the parameter region where the stripe-ordered state with the twofold degeneracy associated with the rotational symmetry of the lattice is stabilized for weaker randomness. This might imply that the SG state is stabilized over the RS state since the state is enabled to adjust to randomness more effectively by employing the additional directional degrees of freedom inherent to the stripe order.

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# Singlet ground state in the spin-1/2 weakly coupled dimer compound $NH_4[(V_2O_3)_2(4,4'-bpy)_2(H_2PO_4)(PO_4)_2]\cdot 0.5H_2O$ .

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We present the synthesis and a detailed investigation of structural and magnetic properties of polycrystalline  $NH_4[(V_2O_3)_2(4,4'-bpy)_2(H_2PO_4)(PO_4)_2]\cdot 0.5H_2O$  by means of x-ray diffraction, magnetic susceptibility, electron spin resonance, and  $^{31}P$  nuclear magnetic resonance measurements. Temperature dependent magnetic susceptibility could be described well using a weakly coupled spin-1/2 dimer model with an excitation gap  $\Delta/k_B \simeq 26.1$  K between the singlet ground state and triplet excited states and a weak inter-dimer exchange coupling  $J'/k_B \simeq 4.6$  K. A gapped chain model also describes the data well with a gap of about 20 K. The electron spin resonance intensity as a function of temperature traces the bulk susceptibility nicely. The isotropic Landé g-factor is estimated to be about  $g \simeq 1.97$ , at room temperature.

We are able to resolve the  $^{31}P$  NMR signal as coming from two inequivalent P-sites in the crystal structure. The hyperfine coupling constant between  $^{31}P$  nucleus and  $V^{4+}$  spins is calculated to be  $A_{\rm hf}(1) \simeq 2963$  Oe/ $\mu_{\rm B}$  and  $A_{\rm hf}(2) \simeq 1466$  Oe/ $\mu_{\rm B}$  for the P(1) and P(2) sites, respectively. Our NMR shift and spin-lattice relaxation rate for both the  $^{31}P$  sites show an activated behaviour at low temperatures, further confirming the singlet ground state. The estimated value of the spin gap from the NMR data measured in an applied field of H=9.394 T is consistent with the gap obtained from the magnetic susceptibility analysis using the dimer model. Because of a relatively small spin gap, NH<sub>4</sub>[(V<sub>2</sub>O<sub>3</sub>)<sub>2</sub>(4,4'-bpy)<sub>2</sub>(H<sub>2</sub>PO<sub>4</sub>)(PO<sub>4</sub>)<sub>2</sub>]·0.5H<sub>2</sub>O is a promising compound for further experimental studies under high magnetic fields. This is a potential quantum magnet in which the Bose Einstein condensation (BEC) can be experimentally realized by the application of magnetic field.

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### Canted antiferromagnetic $120^{\circ}~\mathbf{q}=\mathbf{0}$ order in Sr-Vesignieite.

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We will present the results of  $^{51}V$  NMR, zero applied field  $^{63,65}Cu$  NMR and  $\mu SR$  measurements on powder samples of

Sr-Vesignieite  $SrCu_3V_2O_8(OH)_2$ , a S=1/2 nearly-kagomé Heisenberg antiferromagnet [1]. Our results demonstrate that the ground state is one of  $\mathbf{q}=\mathbf{0}$  antiferromagnetic order with spins canting slightly out of the kagomé plane. We also determine the size of ordered moments and the angle of canting, thereby providing insight into the role of the Dzyaloshinskii-Moriya (DM) interaction which is inevitably present in kagomé systems and tends to induce antiferromagnetic order with a weak ferromagnetic component [2,3].

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# Classical spin nematic phase and spin dynamics in the breathing pyrochlore antiferromagnet $\text{LiGa}_{0.95}\text{In}_{0.05}\text{Cr}_4\text{O}_8$ .

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The A-site ordered spinel chromates  $AA'\mathrm{Cr}_4\mathrm{O}_8$  (i.e.  $A=\mathrm{Li}$ ,  $A'=\mathrm{Ga}$ , In) realize a so-called breathing pyrochlore lattice, where the B site forms a size-alternating array of corner-sharing tetrahedra occupied by  $\mathrm{Cr}^{3+}$  ( $S=\frac{3}{2}$ ) ions. This alternation leads to different exchange interactions, J and J', along the edges of the large and small tetrahedra, respectively. The degree of breathing can be quantified by  $B_f=J'/J$ , whose limiting values 0 and 1 correspond to isolated small tetrahedra and the uniform pyrochlore lattice.

The LiGa<sub>1-x</sub>In<sub>x</sub>Cr<sub>4</sub>O<sub>8</sub> family has proven to manifest a wide range of magnetic behaviours [1-5] as a function of the substitution (and hence bond disorder), x. The end member compositions LiGaCr<sub>4</sub>O<sub>8</sub> ( $B_f = 0.6$ ) and LiInCr<sub>4</sub>O<sub>8</sub> ( $B_f = 0.1$ ) [1] exhibit a series of complex magneto-structural transitions [2,3] resulting in magnetically ordered phases. Recently we have shown that the Néel order is suppressed by even vestigial doping at A' site; for x = 0.05, magnetic order is replaced with a second-order transition to a possible classical spin nematic phase at  $T_f \sim 11$  K [5]. Subsequent inelastic neutron scattering experiments reveal a quasi-elastic response at high temperature, as commonly observed in the pyrochlore antiferromagnets. This is replaced in the low temperature phase by an inelastic mode showing a strong resemblance to the broad resonant mode observed in lightly Cd-doped ZnCr<sub>2</sub>O<sub>4</sub> [6]. The structure factor of the feature is consistent with "weathervane" modes on hexagonal antiferromagnetic loops, which are abundant in the nematic state. The finite energy of the excitation is generated by the biquadratic term in the effective magneto-elastic Hamiltonian, which is also responsible for the onset of the nematic state. These findings provide a unique example of a link between the complex low temperature behaviour and the spin dynamics in chromate spinel system. Furthermore, the spin nematic state might be relevant to similar transitions observed in other doped chromate pyrochlores [6,7].

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## Magnons versus spinons – a numerical study of the 1D-2D dimensional crossover regime of the Heisenberg model.

K. Wohlfeld (University of Warsaw, Poland), K. Jodlowski (University of Warsaw, Poland), A. Klosinski (University of Warsaw, Poland), D. Wlodzynski (University of Warsaw, Poland), P. Wrzosek (University of Warsaw, Poland) — One of the fundamental aspects of highly frustrated magnetism is related to the question whether the frustrated magnet under investigation supports fractional excitations (such as spinons) or its low energy excitations can be well-described in terms of conventional magnons. It turns out that, even for collinear nonfrustrated magnetic systems the answer to such a question is not yet settled [1-3]. In order to get a new physical insight into this problem, here we numerically solve a Heisenberg model in the 1D-2D crossover regime. We show how tuning the interactions between magnons as well as the dimensionality of the system can lead to the changes in the nature of the low-energy excitations.

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#### Topological phases of non-symmorphic crystals: 1/4 filled Shastry-Sutherland lattice.

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Motivated by many Kondo materials which form a Shastry-Sutherland lattice, we investigate possible time-reversal invariant topological insulator of a Shastry Sutherland lattice at quarter filling. At quarter filling, nonsymmorphicity of this system always guarantees gapless electronic state, protecting line degeneracies in the Brillouin zone. In the presence of intrinsic spin-orbit (SO) coupling, we consider the generalized tight-binding model and study the condition for topological insulator where time-reversal and inversion symmetries are preserved but non-symmorphic symmetries are broken. To determine  $Z_2$  invariants, time-reversal invariant momentum (TRIM) points are examined. Furthermore, we also discuss the case of robust degeneracy at M point even with broken symmetries and the appearance of Dirac cones where  $Z_2$  invariant is -1 in the absence of SO coupling.

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#### Pr<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>: when Luttinger semimetal meets Melko-Hertog-Gingras spin ice state.

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We study the band structure topology and engineering from the interplay between local moments and itinerant electrons in the context of pyrochlore iridates. For the metallic iridate  $Pr_2Ir_2O_7$ , the Ir 5d conduction electrons interact with the Pr 4f local moments via the f-d exchange. While the Ir electrons form a Luttinger semimetal, the Pr moments can be tuned into an ordered spin ice with a finite ordering wavevector, dubbed "Melko-Hertog-Gingras" state, by varying Ir and O contents. We point out that the ordered spin ice of the Pr local moments generates an internal magnetic field that reconstructs the band structure of the Luttinger semimetal. Besides the broad existence of Weyl nodes, we predict that the magnetic translation of the "Melko-Hertog-Gingras" state for the Pr moments protects the Dirac band touching at certain time reversal invariant momenta for the Ir conduction electrons. We propose the magnetic fields to control the Pr magnetic structure and thereby indirectly influence the topological and other properties of the Ir electrons. Our prediction may be immediately tested in the ordered  $Pr_2Ir_2O_7$  samples. We expect our work to stimulate a detailed examination of the band structure, magneto-transport, and other properties of  $Pr_2Ir_2O_7$ .

[1] Xu-Ping Yao, Gang Chen, arXiv:1712.06534

#### Hierarchy of exchange interactions in the triangular-lattice spin-liquid YbMgGaO<sub>4</sub>

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The spin-1/2 triangular lattice antiferromagnet YbMgGaO<sub>4</sub> has attracted recent attention as a quantum spin-liquid candidate with the possible presence of off-diagonal anisotropic exchange interactions induced by spin-orbit coupling. Whether a quantum spin-liquid is stabilized or not depends on the interplay of various exchange interactions with

chemical disorder that is inherent to the layered structure of the compound. We combine time-domain terahertz spectroscopy and inelastic neutron scattering measurements in the field polarized state of YbMgGaO<sub>4</sub> to obtain better microscopic insights on its exchange interactions. Terahertz spectroscopy in this fashion functions as high-field electron spin resonance and probes the spin-wave excitations at the Brillouin zone center, ideally complementing neutron scattering. A global spin-wave fit to all our spectroscopic data at fields over 4 T, informed by the analysis of the terahertz spectroscopy linewidths and neutron diffuse scattering, yields stringent constraints on *g*-factors and exchange interactions. Our results paint YbMgGaO<sub>4</sub> as an easy-plane XXZ antiferromagnet with the combined and necessary presence of sub-leading next-nearest neighbor and weak anisotropic off-diagonal nearest-neighbor interactions. Moreover, the obtained *g*-factors are substantially different from previous reports. This works establishes the hierarchy of exchange interactions in YbMgGaO<sub>4</sub> and strongly constrains possible mechanisms responsible for the observed spin-liquid phenomenology.

### Absence of long-range order in K<sub>2</sub>Ni<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> with a novel modified hyper-kagome lattice.

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In recent years several magnetic compounds have been suggested to have a ground state without long-range order. It is assumed that such a state is characterized by a highly dynamic spectra of entangled spins, i.e. a quantum spin liquid. A necessary requirement is a geometrical frustration imposed by the underlying crystal lattice of magnetic ions, paired with antiferromagnetic interactions. Well-known systems are 2D triangular  $NiGa_2S_4$  and  $YbMgGaO_4$ , 2D kagome  $ZnCu_3(OH)_6Cl_2$  and 3D hyper-kagome  $Na_4Ir_3O_8$ . [1]

Here we present results of our investigation of K<sub>2</sub>Ni<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> which belongs to a family of sulphates of the langbeinite type K<sub>2</sub>M<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>, investigated for their ferroelectric behavior [2]. Our susceptibility, μSR, specific heat and neutron diffraction experiments show that no long range order occurs down to lowest temperatures achieved. A linear Curie-Weiss behavior of inverse susceptibility is observed from 350 K down to ~ 50 K, with θ = −17 K, indicating a dominant antiferromagnetic interaction. μSR revealed absence of oscillations or wiggles in a wide temperature range from 300 K down to 20 mK with no sign of frozen moments or any static magnetism emerging from applying a longitudinal field up to 2000 G. Magnetic specific heat (extracted using a non-magnetic analog K<sub>2</sub>Mg<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>) exhibits a broad maximum centered around 5 K with C<sub>P</sub> ~ T<sup>2</sup> for 0.05 < T < 1 K which points to gapless, linearly dispersive modes in two dimensions. Similar finding has been reported for a two-dimensional triangular lattice compound NiGa<sub>2</sub>S<sub>4</sub> [3] but for K<sub>2</sub>Ni<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> it represents a surprising discovery since it crystallizes in a chiral cubic P2<sub>1</sub>3 space group without any distinguished low-dimensional features. In fact, it can be described as a modification of a hyper-kagome lattice in Na<sub>4</sub>Ir<sub>3</sub>O<sub>8</sub>: there are two crystallographic sites (Ni1 and Ni2), each forming a network of equilateral triangles. Triangles are further connected in a non-coplanar way to form pentagons, raising even further the level of geometrical frustration. With Ni ions having S=1 spin state K<sub>2</sub>Ni<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> represents a new route for testing theories of quantum spin liquids beyond S=1/2.

[1] Y. Zhou et al., Rev. Mod. Phys. 89, 025003 (2017) [2] D. Speer and E. Salje, Phys. Chem. Minerals 13, 17 (1986) [3] S. Nakatsuji et al., Science 309, 1697 (2005)

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