MARCH 22-26

21:00-24:00 (JST)
13:00-16:00 (CET)
8:00-11:00 (EDT)

INTERNATIONAL WORKSHOP ON QUANTUM MAGNETS IN EXTREME CONDITIONS

Scope

The Focus of this international workshop is on the fascinating emergent physical properties of solid-state quantum magnets in both theoretical models, computations and predictions, as well as experimental results. The program will center on the effects of dimensionality, geometrical frustration, and symmetry, with an emphasis on extreme materials environment conditions of high magnetic fields, applied pressures, doping, and temperatures.

https://ykohama.issp.u-tokyo.ac.jp/qmec2020/index.html

THE INSTITUTE FOR SOLID STATE PHYSICS
THE UNIVERSITY OF TOKYO

Program

JST	CET	EDT	22nd March Monday	23rd March Tuesday	24th March Wednesday	25th March Thursday	26th March Friday
21:00 – 21:30	13:00 – 13:30	08:00 – 08:30	Opening	6. Henrik M. Rønnow	11. Marcelo Jaime	16. Zenji Hiroi	21. Tsutomu Momoi
21:30 – 22:00	13:30 – 14:00	08:30 – 09:00	1. Frédéric Mila	7. P. Sengupta	12. Alix McCollam	17. Mladen Horvatić	22. Tsuyoshi Okubo
22:00 – 22:30	14:00 – 14:30	09:00 – 09:30	2. Masashi Takigawa	8. P. Corboz	13. Y. Kato	18. Yasuhiro H. Matsuda	23. H. Takeda
22:30 – 23:00	14:30 – 15:00	09:30 – 10:00	3. Takahiro Sakurai	9. Yoshimitsu Kohama	14. Nicolas Laflorencie	19. S. Kimura	24. C. Hotta
23:00 – 23:30	15:00 – 15:30	10:00 – 10:30	4. Anders W. Sandvik	10. A. Saul	15. Adrian E. Feiguin	20. J. L. Musfeldt	25. Christian Rüegg
23:30 – 24:00	15:30 – 16:00	10:30 – 11:00	5. Sara Haravifard	Discussion	Coffee break	Coffee break	Discussion + Closing

The workshop is free of charge. To receive a ZOOM invitation, please register at the conference home page (Registration | Quantum Magnets in Extreme Conditions). Please feel free to encourage students, postdocs, and other collaborators to register and attend QMEC.

Time allocated for presentations is **30 minutes**, with 23-25 minutes for the talk, followed by 5-7 minutes for questions. Due to the workshop busy schedule, we kindly ask all presenters to stay well within the allocated time limits. The workshop will facilitate a clearly visible timer window.

ABSTRACTS

MARCH 22ND

The saga of the Shastry-Sutherland compound $SrCu_2(BO_3)_2$

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Key Words: frustrated magnetism, magnetization plateaus, high magnetic field

Since the discovery of its first magnetization plateaus in 1999, the compound $SrCu_2(BO_3)_2$ has been the focus of considerable and uninterrupted activity. Its arrangement of orthogonal spin-1/2 dimers, soon renamed the Shastry-Sutherland lattice after its first theoretical investigation in the early eighties, induces a strong frustration, and the kinetic energy of the triplet excitations is strongly reduced, leading to a strongly correlated system of hard-core bosons. The physics of this system has proven to be much richer and far more subtle than expected from the well understood toy model of a frustrated ladder. For instance, the plateaus have been argued to be crystals of bound states and not of single triplets. But even in zero field the Shastry-Sutherland model is much richer with three phases (as opposed to one) that should be reachable by applying pressure. This has triggered a tremendous activity aimed at studying the phase diagram of $SrCu_2(BO_3)_2$ in extreme conditions of field and pressure, leading to several surprises and to an amazingly rich phase diagram. In this introductory talk, I will try to give an overview of the fascinating physics of the Shastry-Sutherland model, and of its nearly perfect experimental realization, $SrCu_2(BO_3)_2$.

High pressure phases of the Shastry-Sutherland spin system $SrCu_2(BO_3)_2$

Masashi Takigawa
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Key Words: $SrCu_2(BO_3)_2$, high pressure, symmetry breaking, NMR

The two-dimensional coupled dimer spin system $SrCu_2(BO_3)_2$ is a good realization of the frustrated Shastry-Sutherland model and exhibits a number of fascinating properties. In addition to the series of fractionally quantized magnetization plateaus in high magnetic fields, recent attention has focused on quantum phase transitions in high pressure, which changes the ratio of exchange couplings. In our early ^{11}B NMR experiments in high pressures up to 2.4 GPa (Waki *et al.*, J. Phys. Soc. Jpn. **76** (2007) 073710), the NMR spectra show four-fold splitting of NMR lines, indicating both the structural transition breaking the S_4 symmetry and the doubling of the magnetic unit cell. The later experiments, however, did not show signature of the structural transition but still exhibit line splitting below 4 K, indicating two inequivalent B sites, both of which preserve the mirror symmetry. This result is compatible with the plaquette singlet with the diagonal bonds (full plaquette) but inconsistent with the empty plaquette. We discuss implication of our results in relation to other recent experiments and theories, as well as possible problems concerning the inhomogeneity of pressure (non-hydrostaticity) and pressure calibration.

Development of Multi-extreme THz ESR System and Its Application to Orthogonal Dimer Spin Substance $SrCu_2(BO_3)_2$

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Key Words: ESR, high pressure, THz, plaquette singlet, $SrCu_2(BO_3)_2$

THz ESR measurement under high field and high pressure is a very powerful means for exploring novel physical phenomena of quantum magnetic materials. We have developed a pressure cell which has the high pressure and wide frequency regions to enable ESR measurement under such multi extreme conditions. The pressure cell is of the piston cylinder type, and we use ZrO_2-based ceramic for the internal parts, which has good transmission to electromagnetic waves and toughness. By using these ceramic parts, we achieved the maximum pressure of 2.5 GPa and the wide frequency range of 0.05 – 0.8 THz [1]. It can be combined with various superconducting magnets, and has already succeeded in combining with a cryogen-free magnet with a maximum magnetic field of 25 T [2].

As an application example, we will show the results of $SrCu_2(BO_3)_2$, which is known as the orthogonal dimer spin system. This substance has a characteristic crystal structure in which the S = 1/2 antiferromagnetic dimers are arranged orthogonally to each other in a two-dimensional plane. When the intra- and interdimer interactions are represented by J and J', respectively, the ground state of the system is the dimer singlet state at the limit of J'/ J = 0 while the Néel state at the limit of J'/ J = ∞. On the other hand, a novel quantum state called a plaquette singlet state is theoretically predicted between these two states, and the realization of the quantum phase transition to this plaquette singlet state has long been expected in this system at the ratio J'/ J ~ 0.68 [3]. In recent years, a transition from the dimer singlet phase to a new phase has been observed in this system by applying the pressure.

In our multi extreme ESR measurement for this system, direct transitions from the ground state to the low-lying excited states were observed, and a jump was observed in the excited energy at P = 1.85 GPa [4]. From the detailed analysis, it was found that this pressure corresponds to the ratio J'/ J = 0.66. It shows relatively good agreement with the theoretically predicted ratio (~ 0.68), and we concluded that the observed anomaly in the excited energy corresponds to the quantum phase transition to the plaquette singlet state.

[1] T. Sakurai *et al.*, J. Magn. Reson. **259** (2015) 108. [2] T. Sakurai *et al.*, J. Magn. Reson. **296** (2018) 1. [3] T. Sakurai *et al.*, J. Phys. Soc. Jpn. **87** (2018) 033701. [4] A. Koga and N. Kawakami, Phys. Rev. Lett. **84** (2000) 4461.

On the phase transition between plaquette-singlet and antiferromagnetic phases in $SrCu_2(BO_3)_2$ under high pressure

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Key Words: Shastry-Sutherland material, plaquette-singlet state, antiferromagnet, quantum phase transitions, deconfined quantum criticality

Recent heat capacity measurements have finally located the expected plaquette-singlet (PS) and antiferromagnetic (AF) states in the quasi-2D Shastry-Sutherland (SS) material $SrCu_2(BO_3)_2$ at pressures above 2 GPa and temperatures below 4 K [1]. While the experiments so far have not reached low enough temperatures, below 1 K, to detect the direct transition between the two symmetry-breaking phases, the pressure window has been narrowed down to between 2.5 and 3 GPa. With this information at hand, various experiments will likely soon be able to study the PS–AF transition in detail. This transition is the best candidate to date for an experimental realization of deconfined quantum criticality [2] and related "beyond Landau" phenomena such as weak first-order, spin-flop-like, PS–AF transitions with emergent O(4) symmetry [3].

The SS material is to a good approximation described by the frustrated $S = 1/2$ SS spin model, but the effects of interlayer couplings cannot be neglected when analyzing its PS–AF transition, as pointed out in Ref. [1]. This fact motivates detailed studies of a "designer Hamiltonian" for the 2D PS–AF transition—the checked-board J-Q (CBJQ) model [3]—in the presence of weak interlayer AF couplings. Such modeling is important, in particular, for exploring remnants of emergent O(4) symmetry and DQCP scaling on the expected first-order line of PS–AF transitions at $T \geq 0$, up to the triple point [4]. Unlike the SS model, the CBJQ model is amenable to large-scale, unbiased quantum Monte Carlo simulations, thus allowing detailed studies of many universal aspects of the PS–AF transition. I will discuss this work as well as a recent DMRG study of deconfined quantum criticality in the 2D SS model [5].

References

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3. B. Zhao, P. Weinberg, and A.W. Sandvik, Nat. Phys. **15**, 678 (2019).

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5. J. Yang, A. W. Sandvik, and L. Wang (in preparation).

Phase Diagram of Shastry-Sutherland Compound $SrCu_2(BO_3)_2$ at High-Pressure and High-Field

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Key Words: High-Pressure, High-Field, Shastry-Sutherland.

An understanding of the phase diagrams of quantum magnets is a crucial foundation for exploring and realizing various types of exotic quantum matter. Systems that lie close to phase boundaries are particularly interesting because they can be tuned relatively easily between competing quantum ground states by experimental knobs such as pressure and magnetic field. One notable example is the Shastry-Sutherland 2-D network of interacting spins and its experimental realization, $SrCu_2(BO_3)_2$, which can be driven from a spin-dimer singlet state to a plaquette state by applying a hydrostatic pressure. The exact nature of this plaquette state has been a matter of debate and in particular its magnetic properties have not been studied systemically. Here, we report a comprehensive description of the magnetic phase diagram using both tunnel diode oscillator (TDO) measurements and infinite projected entangled pair states (iPEPS) calculations. Our results establish an intricate evolution of the magnetic plateaus and the plaquette state with high pressure and high field, revealing a rich phase diagram.

Abstracts

MARCH 23rd

Neutron Scattering and Specific Heat Results from the Shastry-Sutherland Compound $SrCu_2(BO_3)_2$ Under Pressure

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Key Words: Neutron Scattering; Specific Heat; Quantum Phase Transition

I will present multiple recent experimental results on the Shastry-Sutherland compound $SrCu_2(BO_3)_2$, including: Neutron scattering and specific heat data from the 4-spin plaquette singlet phase above 20kbar[1,2]; Unusual damping mechanism at finite temperature[3]; and attempts to access the 1/8 plateau phase by combining 26T magnetic field and 12 kbar pressure.

[1] M. Zayed et al., Nature Physics 13 962 (2017)
[2] J. Larrea Jimenez, Nature *in press*
[3] M. Zayed et al., Phys. Rev. Lett. 113 067201 (2016)

Weyl-triplons in $SrCu_2(BO_3)_2$

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Key Words: Geometric frustration, Shastry-Sutherland, topological excitations.

We show that Weyl triplons are expected to appear in the low energy magnetic excitations in the canonical Shastry-Sutherland compound, $SrCu_2(BO_3)_2$, a quasi-2D frustrated quantum magnet. Our results show that when a minimal, realistic inter-layer coupling is added to the well-established microscopic model describing the individual layers, Dirac points that appear in the zero-field triplon spectrum of the 2D model splits into two pairs of Weyl points along the k_z direction. Varying the strength of the inter-layer DM interaction and applying a small longitudinal magnetic field results in a range of band topology transitions accompanied by changing numbers of Weyl points. We propose inelastic neutron scattering along with thermal Hall effect as the experimental techniques to detect the presence of Weyl-node in the triplon spectrum of this material.

Tensor network study of $SrCu_2(BO_3)_2$ under pressure

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Key Words: Frustrated magnetism, tensor network methods, quantum spin systems, phase transitions

The frustrated quantum antiferromagnet $SrCu_2(BO_3)_2$ constitutes a realization of the paradigmatic Shastry-Sutherland model and exhibits a very rich phase diagram as a function of pressure and magnetic field. In this talk I report on recent progress in the numerical study of this model using two-dimensional tensor network algorithms, which have recently been extended to finite temperature. We find a close agreement between the experimental and numerical data for the specific heat, revealing a sharp peak at

pressures between 18-20 kbar. We show that this feature corresponds to a finite-temperature critical point, analogous to the critical point of water, which terminates the first order line emanating from the discontinuous quantum phase transition between the dimer and plaquette phase at zero temperature. We numerically confirm that this critical point is compatible with the expected 2D Ising universality class.

Entropy near the magnetization plateau of $SrCu_2(BO_3)_2$

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Key Words: High Magnetic Field, Shastry-Sutherland, Specific Heat, Magnetocaloric Effect

$SrCu_2(BO_3)_2$ is an exciting material that shows the sequence of magnetization plateaux and possible supersolid states under high magnetic fields [1,2]. The plateaux are well described by the crystallization of the triplets (S_z = 1), while the supersolid state is pictured as the superposition of a magnetic crystal and a Bose-Einstein condensate of the triplets. It is also theoretically predicted that $SrCu_2(BO_3)_2$ shows the condensate/crystallization of the other bosonic quasi-particles, quintuplet bound state with S_z = 2 [4,5,6]. An ESR study clearly indicates the existence of the S_z = 2 state below 27 T [7], but the crystallization and/or Bose-Einstein condensation of the S_z = 2 state have yet to be experimentally observed.

In this research, we have investigated the temperature dependence of the magnetic entropy in $SrCu_2(BO_3)_2$ up to 30 T by using specific heat [8] and magnetocaloric effect measurements [9]. Our study reveals the emergence of a broad anomaly in C_p and large magnetic entropy in the intermediate field range from 24 to 27 T. This anomaly can neither be attributed to the 1st order phase transition to the magnetization plateau nor Schottky anomaly [10]. Since there is no internal field observed in NMR [1] for the intermediate field range, we currently interpret these anomalies as the crystallization or Bose-Einstein condensation of the S_z = 2 state.

[1] K. Kodama et al., *Science* **298**, 395-399 (2002).
[2] M. Takigawa et al., *Phys. Rev. Lett*. **110**, 067210 (2013).
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[10] Hiroyuki Tsujii et al., *J. Phys. Soc. Jpn*. **80**, 043707 (2011).

Magnetoelastic interaction in the two-dimensional magnetic material $MnPS_3$ studied by first principles calculations and Raman experiments

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Key Words: Magnetic phase transition, Raman scattering, Heisenberg model, Density functional theory, $MnPS_3$, Antiferromagnetism

$MnPS_3$ belongs to a large family of two-dimensional (2D) transition-metal chalcogenophosphates MPX_3 (M = V, Cr, Mn, Fe, Co, Ni, Cu, Zn, and X = S, Se, Te) showing stacking properties characteristic of the van-der Waals materials while possessing magnetic order.

In this work we report experimental and theoretical studies on the magnetoelastic interactions in $MnPS_3$. Raman scattering response measured as a function of temperature shows a blue shift of the Raman active modes at 120.2 and 155.1 cm^{-1}, when the temperature is raised across the antiferromagnetic-paramagnetic transition.

Density functional theory (DFT) calculations have been performed to estimate the effective exchange interactions and calculate the Raman active phonon modes. The calculations lead to the conclusion that the peculiar behavior with temperature of the two low energy phonon modes can be explained by the symmetry of their corresponding normal coordinates which involve the virtual modification of the super-exchange angles associated with the leading antiferromagnetic (AFM) interactions.

Abstracts

MARCH 24th

Field-dependent thermal, magnetic, and lattice properties of the quantum spin liquid candidate α-$RuCl_3$

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Key Words: Quantum spin liquid, magnetocaloric effect, magnetostriction, Kitaev model, pulsed magnetic fields.

I will summarize recent results[1] on magnetocaloric, thermal expansion, and magnetostriction data in α−$RuCl_3$ single crystals that help to better understand its temperature-field phase diagram and uncover the magnetic-field dependence of an apparent energy gap structure Δ(H) that evolves when the low-temperature antiferromagnetic order is suppressed. Remarkably, our magnetocaloric effect data provide, below 1 K, unambiguous evidence for dissipative phenomena at Hc, a smoking gun for a first-order phase transition. Conversely, our results show little support for a phase transition from a QSL to a polarized paramagnetic state above Hc. The emergent physical picture will be discussed in the context of an extensive body of experimental results on this puzzling quantum spin liquid candidate available in the literature.

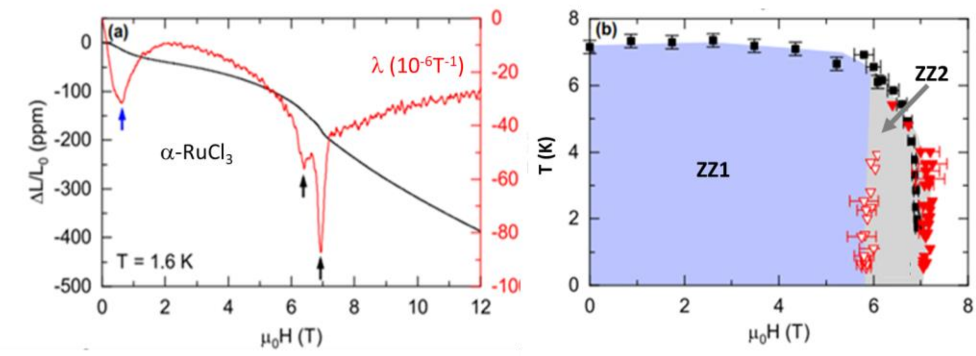

Figure 1: ***(a)*** *Strain $\Delta L/L_0 = (L-L_0)/L_0$ in parts per million, and magnetostriction $\lambda = \partial(\Delta L/Lo)/\partial H$, vs magnetic field measured at T = 1.6K showing two sharp anomalies in the 6-7T field range corresponding to the suppression of antiferromagnetic zig-zag phases ZZ1 and ZZ2. (b) (T,H) phase diagram from anomalies in the magnetocaloric effect, thermal expansion, and magnetostriction results.*

References

[1] R. Schonemann, S. Imajo, F. weickert, J. Yan, D.G. Mandrus, Y. Takano, E.L. Brosha, P.F.S. Rosa, S.E. Nagler, K. Kindo, and M. Jaime. *Phys. Rev. B* **102**, 164544 (2020).

The high field Fermi surface of $CeRhIn_5$

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Key Words: Heavy fermions, Fermi surface, high magnetic field.

$CeRhIn_5$ is an important material in the context of quantum criticality, as it hosts two accessible quantum critical points where antiferromagnetism is suppressed by applied pressure and by high magnetic field, respectively. The high pressure quantum critical point is established to be of the Kondo destruction type, associated with delocalisation of the Ce *f*-electron and an abrupt transition in the size and shape of the Fermi surface as the pressure is increased [1]. The high magnetic field quantum critical point is less well understood, but has been proposed to take place at $B_C \sim 50$ T, following an *f*-electron delocalisation transition that takes place within the antiferromagnetic state at ~ 30 T [2].

We have recently re-examined the high field Fermi surface of $CeRhIn_5$ using de Haas-van Alphen oscillations measured via torque magnetometry in magnetic field up to 70 T. In particular, we have examined the detailed angle-dependence of the oscillations to follow the shape of specific branches of the Fermi surface. Our results suggest that the 30 T transition in $CeRhIn_5$ does not represent delocalisation of the *f*-electron, and that the *f*-electrons remain localised, corresponding to a "small" and unchanged Fermi surface across the quantum critical point and to the highest fields measured [3].

I will present our quantum oscillation data, and the conclusions that can be drawn about the high field phase diagram of $CeRhIn_5$. I will also highlight some features in the high field data that have yet to be understood.

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[2] L. Jiao *et al*., Proc. Natl. Acad. Sci. USA **112**, 673 (2015).
[3] S. Mishra, *et al*. Physical Review Letters. **126**, 016403 (2021).

Magnetic-field-induced tunability of magnon bound states: Scattering resonances and Efimov states in $Yb_2Ti_2O_7$

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Key Words: Magnon, Efimov effect, Pyrochlore oxcide.

In 1970, Efimov predicted the emergence of a sequence of three-body bound states when the strength of attractive force between two particles is about to reach the resonant condition. These "Efimov" states were observed in 2006 using an ultracold gas of ^{133}Cs atoms, where the inter-atomic interactions are controlled by the Feshbach resonance technique. In 2012, we proposed that Efimov states can also be realized in magnetic materials as three-magnon bound states and provided numerical estimates of the binding energies for various models with typical collinear magnetic orderings [1]. However, no candidate material for realizing the unitary limit of two magnons has been found so far mainly because of the limited tunability of the Hamiltonian parameters of real quantum magnets. We will demonstrate that an external magnetic field can also be used to tune the magnon scattering length in quantum ferromagnets with strong spin-orbit coupling. The two-magnon resonant condition can then be achieved in $Yb_2Ti_2O_7$ by applying a field of ~13 T along the [110] direction, which leads to the formation of Efimov states in the three-magnon spectrum [2]. We will see that the same principle can be applied to other quantum ferromagnets with strong spin-orbit coupling.

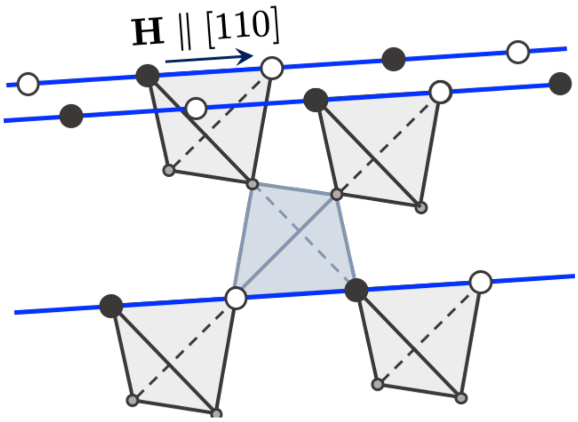

Figure 1: Pyrochlore lattice formed by magnetic ions.

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Disorder-Induced Revival of Bose-Einstein Condensation in the Quantum Magnet DTNX at High Magnetic Fields

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Key Words: Disorder, coupled S=1 chains, high-magnetic field

The high magnetic field regime of the disordered (Br-doped) quasi-one-dimensional S=1 antiferromagnetic material DTNX, $Ni(Cl_{(1-x)}Br_x)_2$ — $4SC(NH_2)$, was believed to provide the first experimental realization of the elusive Bose-Glass phase in a quantum magnet [1]. However, our recent experimental and theoretical works [2-5] revealed a much richer scenario where impurity-induced localized bosonic degrees of freedom (building blocks for the putative Bose-Glass) form a new kind of Bose-Einstein condensate at low temperature: the BEC* phase (Fig. 1). This is a purely many-body effect where interactions and disorder cooperate to restore a phase coherence via an "order-by-disorder" mechanism [6].

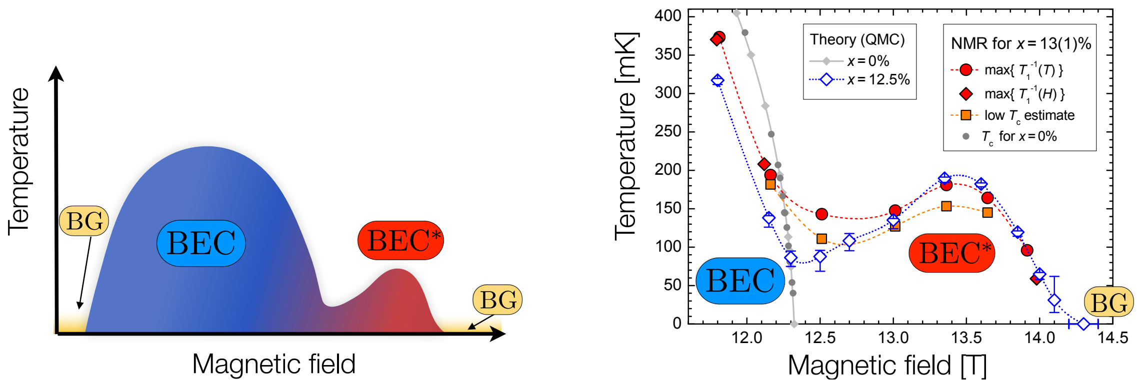

Figure 1. Left: Sketch of the global phase diagram of DTNX, where colors denote the BEC (blue) and BEC* (red) phases, and the Bose-glass (BG, yellow) regime. Right: Focus on the higher field regime. The critical temperature determined from quantum Monte Carlo simulations for x=12.5 % doping (blue open diamonds) is compared to Tc estimates from $1/T_1$ NMR data in an x=13(1) % doped sample. Adapted from [5].

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A time-dependent approach to inelastic scattering spectroscopies in and away from equilibrium: beyond perturbation theory

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Key Words: DMRG, INS, ARPES, RIXS, spectroscopies.

I present a new computational paradigm to simulate time and momentum resolved inelastic scattering spectroscopies in correlated systems. The conventional calculation of scattering cross sections relies on a treatment based on time-dependent perturbation theory, that provides formulation in terms of Green's functions. In equilibrium, it boils down to evaluating a simple spectral function equivalent to Fermi's golden rule, which can be solved efficiently by a number of numerical methods. However, away from equilibrium, the resulting expressions require a full knowledge of the excitation spectrum and eigenvectors to account for all the possible allowed transitions, a seemingly unsurmountable complication. Similar problems arise when the quantity of interest originates from higher order processes, such as in Auger, Raman, or resonant inelastic X-ray scattering (RIXS). To circumvent these hurdles, we introduce a time-dependent approach that does not require a full diagonalization of the Hamiltonian: we simulate the full scattering process, including the incident and outgoing particles (neutron, electron, photon) and the interaction terms with the sample, and we solve the time-dependent Schrödinger equation. The spectrum is recovered by measuring the momentum and energy lost by the scattered particles, akin an actual energy-loss experiment. The method can be used to study transient dynamics and spectral signatures of correlation-driven non-equilibrium processes, as I illustrate with several examples and experimental proposals using the time-dependent density matrix renormalization group method as a solver. Even in equilibrium, we find higher order contributions to the spectra that can potentially be detected by modern instruments.

Abstracts

MARCH 25th

Dimensional Reduction by Geometrical Frustration

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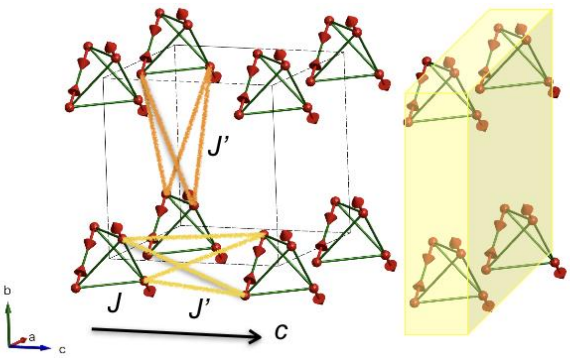
Key Words: dimensional reduction, geometrical frustration, pharmacosiderite

Dimensionality is one of the most important factors that critically govern phase transitions and elementary excitations in solids. Low dimensional spin systems are approximately materialized in actual three-dimensional (3D) crystals via anisotropic chemical bonding. However, dimensionality may not be always a "built-in" character of a crystal structure but can be an emergent property in a frustrated spin system. One example is found in $BaCu_2Si_2O_6$, in which BEC of triplons takes an essentially 2D character near a quantum critical point between the gapped state and long-range order [1]. This is ascribed to a geometrical frustration between neighboring square lattices that stack in a staggered manner so as to cancel the inter-layer couplings. Thus, true two-dimensionality seems to be preserved by frustration in the 3D lattice.



Here we discuss on "dimensional reduction" by geometrical frustration in two spin systems. In $Ca_3ReO_5Cl_2$ comprising an anisotropic triangular lattice (ATL) made of spin-1/2 Re^{6+} ions, one dimensionalization is clearly evidenced by magnetic susceptibility and heat capacity measurements, in spite that the inter-chain zigzag coupling is significantly large: J'/J = 0.42 [2]. Further interesting dimensional reduction was recently observed in a synthetic iron mineral, pharmocosiderite $(H_3O)Fe_4(AsO_4)_3(OH)_4$•$5.5H_2O$ [3]. It comprises tetrahedral clusters made of spin-5/2 Fe^{3+} ions in a cubic primitive cell, as depicted in the figure. The antiferromagnetic Heisenberg interactions are determined as J = 10.6 K and J' = 2.9 K. A q = 0, Γ_5 order sets in at 6 K, in which a 2D spin fluctuation is observed. This is ascribed to a two dimensionalization by frustration only for the J' tetrahedral coupling along the *c* axis. It is emphasized that, compared with the ATL antiferromagnets, the resulting 2D anisotropy is not fixed to the crystal lattice but is induced by the evolution of magnetic correlations towards the LRO.

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Distinguishing dimensionality of a spin system: determination of the Tomonaga-Luttinger parameter *K* in quasi-1D systems

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Keywords: Antiferromagnets, Tomonaga-Luttinger liquid, Spin dynamics, NMR.

The nuclear magnetic resonance (NMR) in antiferromagnetic quantum spin materials has recently provided a major result regarding quasi-one-dimensional (quasi-1D) systems, namely an important improvement of the standard, "Tomonaga-Luttinger liquid" (TLL), low-energy description of these systems in their gapless regime (typically induced by magnetic field). This purely 1D description is characterized by power-law dependence of the response/correlation functions, whose exponents are defined by the TLL parameter *K*. However, at low temperature the effects of 3D exchange couplings significantly modify the TLL response, which can be theoretically described by a random phase approximation (RPA). We confirm the validity of the recently derived RPA correction for the spin-spin correlation functions [1], by applying this formula to the temperature dependence of the NMR relaxation rate T_1^{-1} in the two representative quasi-1D spin compounds, $(C_7H_{10}N)_2CuBr_4$ (DIMPY) and $BaCo_2V_2O_8$. A successful fit of the T_1^{-1} data thus provided the first direct experimental determination of the *K* values that perfectly agrees with the theoretically calculated ones [2].

In general, by taking into account the RPA correction, we strongly broaden the scope of the TLL description, which becomes applicable to less quasi-1D compounds/systems approaching the 3D regime. The RPA correction can be easily calculated for any geometry of the 3D exchange couplings, and provides a $T_1^{-1}(T)$ dependence that is clearly different from those observed in either quasi-2D or in 3D spin systems. NMR T_1^{-1} data thus provide an exceptionally simple way to distinguish the effective dimensionality of a gapless spin system. In quasi-1D systems, from T_1^{-1} data we directly determine the *K* parameter, providing insight in the nature and the strength of quasiparticle interactions.

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Metastable magnetization plateau states observed in an $S = 1$ two-leg spin ladder by fast sweeping of a magnetic field up to 150 T

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Key Words: Spin ladder, Magnetization plateau, High magnetic field

The entire magnetization process in the S =1 two-leg organic spin ladder BIP-TENO [1] has been studied with an ultrahigh magnetic field of up to 150 T. Nontrivial multiple magnetization plateaus are observed, indicating there exist strong quantum correlation between spins. A magnetization curve obtained up to 100 T is shown in Fig.1. In addition to the previously reported 1/4 plateau [2], another nontrivial 1/3 plateau appears only when spins behave adiabatically being decoupled to the lattice degree of freedom. A novel spontaneous symmetry breaking occurs with the spin-lattice decoupling induced by a fast evolution of external magnetic fields in the range of μs. Under the adiabatic condition, five fractional (1/4, 1/3, 1/2, 2/3, 3/4) magnetization plateau states are likely to appear and the magnetization seems to saturate at around 150 T.

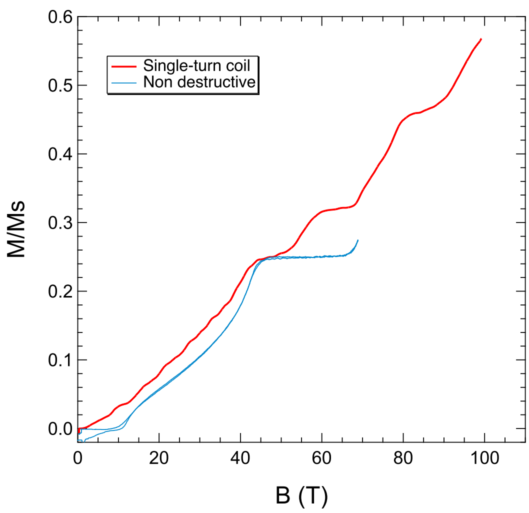

Figure 1. Magnetization process of a single crystal of BIP- TENO measured with the μs single-turn coil at 4.2 K up to 100 T (red curve). The light-blue curve shows the magnetization process of another single crystal of BIP-TENO with a non-destructive ms pulsed magnet at 1.3 K [2].

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Multiferroic Behaviors in the Quantum Spin Dimer System

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Key Words: quantum spin dimer, magnetoelectric effect, multiferroics

The quantum spin dimer system $TlCuCl_3$ with S = 1/2 is known to show the magnetic-field-induced antiferromagnetic ordering owing to Bose-Einstein condensation of magnon quasiparticles [1]. An important feature of a quantum spin dimer is that there are finite matrix elements of a vector spin chirality $\boldsymbol{S}_l \times \boldsymbol{S}_r$ between the spin singlet and triplet states. Reflecting this feature, $TlCuCl_3$ shows ferroelectiricity in the magnon BEC phase, of which ground state wave function can be described by superposition of the singlet and triplet states [2]. Thus, the ordered phase in $TlCuCl_3$ is multiferroic state. The ferroelectricity in $TlCuCl_3$ is very susceptible to the applied pressure, which suppress the quantum fluctuation inherent in the spin dimer. The application pressure largely expands the ordered state in the temperature-field phase diagram, and also the soft ferroelectriciy of $TlCuCl_3$ becomes harder under higher pressure [3]. The quantum spin dimer shows not only static but also dynamic magnetoelectric effect. The electric dipole transition from the singlet ground to the excited triplet states in the low field phase is possible owing to the magnetoelectric coupling, generated by the vector spin chirality [4]. Furthermore, in the magnon BEC phase, nonreciprocal directional dichroism, for which the strength of the electromagnetic wave absorption changes by reversal of the light propagation direction, has been observed for the microwave excitation of the Nambu-Goldstone mode [5].

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Phase diagram, magnetoelectric coupling, and spin-lattice interactions in multiferroic $(NH_4)_2[FeCl_5\cdot(H_2O)]$

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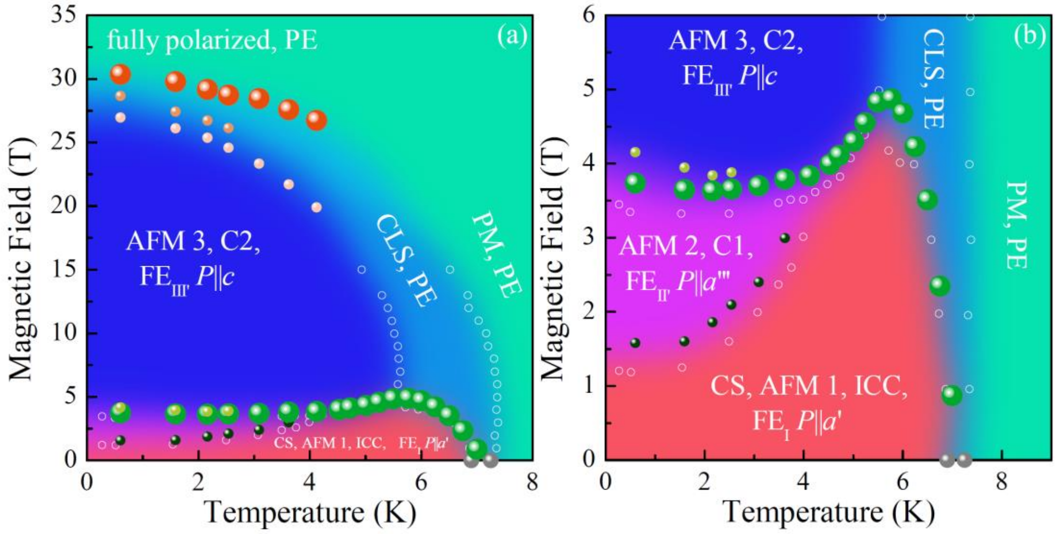
Key Words: magnetization, magnetoelectric coupling, spin-phonon coupling, molecular multiferroic, hydrogen- and halogen bonding, $H – T$ phase diagram

We combine high field polarization, magneto-infrared spectroscopy, and lattice dynamics calculations with prior magnetization work to explore the properties of $(NH_4)_2[FeCl_5\cdot(H_2O)]$ - a molecular multiferroic in which the mixing between charge, structure, and magnetism is controlled by through-space hydrogen- and halogen-bonding interactions. Electric polarization is sensitive to the various field-induced spin reorientations, increasing with field before collapsing to zero across the quasi-collinear to collinear-sinusoidal reorientation due to the restoration of inversion symmetry. Peaks in the magnetoelectric current confirm that the system is a high field multiferroic with strong magnetoelectric coupling - on the order of 0.025 or 0.048 $nC/cm^2\cdot T$ depending on the field regime. Other forms of cross-coupling are active in $(NH_4)_2[FeCl_5\cdot(H_2O)]$. Magneto-infrared spectroscopy reveals that nearly all of the vibrational modes below 600 cm^{-1} are sensitive to the field-induced transition to the fully saturated magnetic state. We analyze these local lattice distortions and use their frequency shifts to extract spin-phonon coupling constants for the Fe-O stretch, Fe-OH_2 rock, and NH_4^+ twist. Examination also uncovers subtle symmetry breaking of the water ligand and ammonium counterion across

the ferroelectric transition. The coexistance of such varied mixing processes in a platform in which interactions are based upon intermolecular hydrogen- and halogen-bonds opens the door to greater understanding of multiferroics and magnetoelectrics governed by through-space interactions.



Abstracts

MARCH 26th

Coupled Trimer Description of Kagome Compound Volborthite

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Key Words: Kagome, Spin nematic, Trimer, Dzyaloshinskii-Moriya interaction, Thermal Hall effect.

Volborthite offers a stimulating example of a frustrated quantum magnet. It contains both ferromagnetic and antiferromagnetic interactions on anisotropic kagome layers. A recent density functional theory calculation has provided a magnetic model based on coupled trimers [1]. This model shows a broad 1/3-magnetization plateau, which is consistent with the experimentally observed plateau behavior. This model also presents a scenario for the appearance of a spin nematic phase below the 1/3 plateau phase. Recently, we further study the effects of Dzyaloshinskii-Moriya (DM) interactions [2], deriving a spin model of S=1/2 pseudospins on trimers. We show that, for a magnetic field perpendicular to the kagome layer, magnon excitations from the 1/3-plateau feel a Berry curvature due to the DM interactions, giving rise to a thermal Hall effect. A comparison with the experiment suggests that the one-dimensionality is stronger than the previous estimation of exchange couplings. Based on this picture, we further analyze low-temperature magnetic phase diagrams.

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Large spin fluctuation in the magnetization process of frustrated square lattice Heisenberg magnets

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Key Words: Frustration, Tensor network, Quantum spin systems

Many exciting phenomena, including non-collinear magnetic orders, magnetization plateaus, and spin liquids, occur in the frustrated spin systems. Such frustrated interactions often appear in geometrically frustrated lattices, such as triangular, kagome, or pyrochlore lattices. In addition to these lattices, when we consider further neighbor interactions or a combination of ferromagnetic and antiferromagnetic interactions, frustrations can happen even in the square lattice. Several organic compounds that can be considered as frustrated square lattice magnets have been reported [1,2].

In this talk, motivated by these compounds, we discuss the nature of S=1/2 square lattice Heisenberg magnets with ferromagnetic and antiferromagnetic nearest-neighbor interactions. To investigate the magnetization process of the model numerically, we employed the infinite tensor product state (iTPS) ansatz for the ground state wave function. We show that in the model corresponding to the compound [1], a part of the spins reveals strong spin fluctuation around the half of saturation magnetization, consistent with experimental observations [1]. The origin of such strong spin fluctuation is explained by a spin-singlet formed by spins connected through strong antiferromagnetic interaction. By varying the interaction strength, we show that such spin fluctuation is related to the 1/2 magnetization plateau stabilized in the vicinity of the model.

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Pressure induced phase transition in the J_1-J_2 square lattice antiferromagnet $RbMoOPO_4Cl$

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Key Words: Frustration, High pressure, NMR.

For the past decades, great efforts have been devoted to discover novel quantum disordered states in frustrated spin systems [1, 2]. One of the key concepts is the geometrical frustration inherent in triangle-based structures such as triangular, Kagome and pyrochlore lattices. In these lattices, exchange interactions on equivalent bonds compete strongly to destabilize magnetic order and may lead to quantum disordered ground states such as spin liquid or spin ice. Another type of frustration can be caused by competition between inequivalent exchange interactions, for example, those on the nearest-neighbor (NN) and the next-nearest-neighbor (NNN) bonds.

In this presentation, we report results of magnetization and ^{31}P NMR measurements under high pressure up to 6.4 GPa on $RbMoOPO_4Cl$, which is a frustrated square-lattice antiferromagnet with competing NN and NNN interactions [3, 4]. Anomalies in the pressure dependences of the NMR shift and the transferred hyperfine coupling constants indicate a structural phase transition at 2.6 GPa, which is likely to trigger significant change of the exchange interactions. In fact, the NMR spectra in magnetically ordered states reveal a change from the columnar antiferromagnetic (CAF) order below 3.3 GPa to the Neel antiferromagnetic (NAF) order above 3.9 GPa. The spin lattice relaxation rate $1/T_1$ also indicates a change of dominant magnetic fluctuations from CAF-type to NAF-type with pressure. Although the NMR spectra in the intermediate pressure region between 3.3 and 3.9 GPa show coexistence of the CAF and NAF phases, a certain component of $1/T_1$ shows paramagnetic behavior with persistent spin fluctuations, leaving possibility for a quantum disordered phase. The easy-plane anisotropy of spin fluctuations with unusual nonmonotonic temperature dependence at ambient pressure gets reversed to the Ising anisotropy at high pressures. This unexpected anisotropic behavior for a spin 1/2 system may be ascribed to the strong spin-orbit coupling of Mo-4*d* electrons.

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Origin of exotic trimerized charge order in 5*d* pyrochlore electronic system with strong spin-orbit coupling

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Key Words: 5d electron, spin-orbit coupling, charge order

We theoretically clarify the origin of the emergent trimerized charge ordering recently found in the β-pyrochlore oxide CsW_2O_6 [1]. The electronic system in this material is understood by considering the lowest Kramers doublet of the $W^{5.5+}$ions, which carries the momentum J_{eff}=1/2, and comes out as the mixtures of t_{2g} triplet after considering the strong spin-orbit coupling (SOC) typical of the 5*d* electrons in a crystal field (Fig1(a)).The resultant band structures are the pyrochlore ones at quarter-filling, and are strongly modified by the SU(2) gauges generated from the SOC. This modification gives rise to a particular type of localized orbitals which serve as exact eigen states of the Hamiltonian including the on-site and nearest neighbor Coulomb interactions, *U* and *V*. The trimerized charge ordering occurs based on these localized orbitals by perfectly excluding 1/4 of the pyrochlore sites. This can be regarded as the self-organization of lattice structure from the pyrochlore to the hyper-kagome (Fig.1(b)) by the interplay of strong SOC and electronic correlation. Some theoretical proofs and the topological quantities of the emergent phase will be discussed.

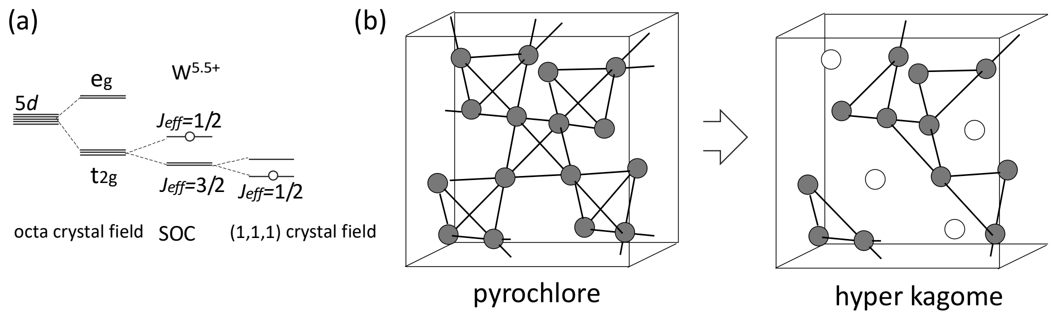

Figure1 (a) Energy levels of 5d-orbitals of an isoated $W^{5.5+}$ion in a crystal field by the octahedral O-ions and with strong SOC. (b) Self organization of electronic states from the metallic state(including topological insulator) on a pyrochlore lattice to the trimierized charge order forming a hyper kagome structure.

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Unconventional Criticality in a Frustration-free, Multi-bilayer Quantum Dimer System

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Key Words: Quantum Magnetism, Neutron Spectroscopy, Quantum Phase Transition.

The dimerized quantum magnet $BaCuSi_2O_6$ was proposed as an example of "dimensional reduction" arising near the magnetic-field-induced quantum critical point (QCP) due to perfect geometrical frustration of its inter-bilayer interactions. We demonstrate by high-resolution neutron spectroscopy experiments that the effective intra-bilayer interactions are ferromagnetic, thereby excluding frustration. We explain the apparent dimensional reduction by establishing the presence of three magnetically inequivalent bilayers, with ratios 3:2:1, whose differing interaction parameters create an extra field-temperature scaling regime near the QCP with a non-trivial but non-universal exponent. We demonstrate by detailed quantum Monte Carlo simulations that the magnetic interaction parameters we deduce can account for all the measured properties of $BaCuSi_2O_6$, opening the way to a quantitative understanding of non-universal scaling in any modulated layered system.

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