

# 物性研究所セミナー

標題：国際強磁場科学セミナー：2017 年度第 4 回：High-field magnetism in the heavy-fermion materials  
CeRh<sub>2</sub>Si<sub>2</sub> and URu<sub>2</sub>Si<sub>2</sub>

日時：2017 年 10 月 2 日(月) 午後 2 時～

場所：物性研究所本館 6 階 第 2 セミナー室 (A612)

講師：Dr. William Knafo

所属：Laboratoire National des Champs Magnétiques Intenses (LNCMI), Centre National de la Recherche Scientifique (CNRS), フランス

## 要旨：

Extreme conditions of intense magnetic field and high pressure are powerful tools to tune the microscopic interactions and explore the magnetic phase diagrams of strongly-correlated electrons systems, as heavy-fermion magnets.

An introduction to the LNCMI-Toulouse pulsed field facility will be given, with a focus on recent technical advances, as the generation of non-destructive pulsed fields up to 99 T, the combination of pulsed fields up to 60 T and high pressures up to 4 GPa, and the possibility to perform neutron diffraction under long-duration pulsed fields up to 40 T. Then I will show recent experimental studies performed using these new setups.

In a first part [1-3], I will present an investigation of the three-dimensional pressure - magnetic field - temperature phase diagram of the heavy-fermion antiferromagnet CeRh<sub>2</sub>Si<sub>2</sub> thanks to our new pressure cells. This phase diagram shows a temperature- and pressure-dependent decoupling of the critical and pseudo-metamagnetic fields, at the borderlines of antiferromagnetism and strongly-correlated paramagnetism. It is representative of a class of heavy-fermion Ising antiferromagnets, where long-range magnetic ordering is decoupled from a maximum in the magnetic susceptibility. Recent neutron diffraction results obtained in phase AF3 between 25.5 and 26 T (at ambient pressure) will also be shown.

In a second part [4-5], I will present a neutron diffraction study - with our new 40-T magnet - of URu<sub>2</sub>Si<sub>2</sub>. This paramagnetic system is well-known for its mysterious “hidden-order” phase, which develops below  $T_0 = 17.5$  K, and can be destabilized under pressure or high magnetic field. We have shown that a spin-density wave is stabilized under a high magnetic field from 35 to 39 T applied along *c*. The interplay between the hidden order, the magnetic and Fermi surface properties of URu<sub>2</sub>Si<sub>2</sub> will be discussed.

These works have been done in collaboration with Dai Aoki, Fabienne Duc, Frédéric Bourdarot, Rikio Settai, Daniel Braithwaite, Keitaro Kuwahara, Hiroyuki Nojiri, Naveen Kumar, Shuhei Kurahashi, Julien Billette, Paul Frings, Xavier Tonon, Eddy Lelièvre-Berna, Louis-Pierre Regnaut and Jacques Flouquet.

## References:

1. “Development of Bridgman-Type Pressure Cell for Pulsed High Magnetic Field”, R. Settai, W. Knafo, D. Braithwaite, S. Kurahashi, D. Aoki, and J. Flouquet, *Review of High Pressure Science and Technology / Koatsuryoku No Kagaku To Gijutsu* 25, 325 (2015).
2. “Pressure cell for transport measurements under high pressure and low temperature in pulsed magnetic fields”, D. Braithwaite, W. Knafo, R. Settai, D. Aoki, S. Kurahashi, and J. Flouquet, *Rev. Sci. Instrum.* 87, 023907 (2016).
3. “Three-dimensional critical phase diagram of the Ising antiferromagnet CeRh<sub>2</sub>Si<sub>2</sub> under extreme conditions of pressure and magnetic field”, W. Knafo, R. Settai, D. Braithwaite, S. Kurahashi, D. Aoki, and J. Flouquet, *Phys. Rev. B* 95, 014411 (2017).

4. “Field-induced spin-density wave beyond hidden order in URu2Si2”, W. Knafo, F. Duc, F. Bourdarot, K. Kuwahara, H. Nojiri, D. Aoki, J. Billette, P. Frings, X. Tonon, E. Lelièvre-Berna, J. Flouquet, and L.-P. Regnault, Nature Commun. 7, 13075 (2016).

標題：量子物質セミナー：Quantum spin liquid in honeycomb iridates  $\text{H}_3\text{LiIr}_2\text{O}_6$  : low temperature specific heat studies

日時：2017年10月2日(月) 午後1時30分～午後2時30分

場所：物性研究所本館6階 第5セミナー室 (A615)

講師：Yosuke Matsumoto

所属：Max Planck Institute for Solid State Research, Department of Quantum Materials (Takagi group)

要旨：

Recently, layered spin-orbit Mott insulators with two-dimensional (2D) honeycomb lattice attract a lot of attention because of possible quantum spin liquid (QSL) states. In particular, Kitaev model, which is a bond dependent Ising model on a honeycomb lattice provides an unique example of an exactly soluble 2D model with topological QSL ground state and fractionalized excitations [1]. Surprisingly, this rather artificial setting, *i.e.*, the bond dependent Ising interactions, has been suggested to be realized in honeycomb iridates composed of edge-sharing  $\text{IrO}_6$  octahedra [2]. Here, the unique  $J_{\text{eff}} = 1/2$  state arising from the strong spin-orbit interaction of  $\text{Ir}^{4+}$  ion is the key ingredient.

While all the candidates suggested so far, such as a- $\text{A}_2\text{IrO}_3$  ( $A = \text{Li}, \text{Na}$ ) and b- $\text{Li}_2\text{IrO}_3$ , magnetically order at finite temperatures [3-5], a recently developed new compound  $\text{H}_3\text{LiIr}_2\text{O}_6$  turned out to be a promising candidate of QSL on a honeycomb lattice [6]. Magnetic susceptibility and  $^7\text{Li}$ -,  $^1\text{H}$ -NMR measurements do not indicate any anomaly down to 0.5 K in spite of the large Weiss temperature  $q_w \sim -90$  K. NMR spectra are quite sharp with a width of about 0.001 mB and exhibit no broadening on cooling demonstrating the cleanest spin liquid ever observed. Both Knight shift and  $1/(T_1T)$  suggest the existence of gapless excitations. Especially, almost constant  $1/(T_1T)$  in weak magnetic fields below 20 K resembles Korringa law inherent to Fermi liquid.

Here I further present the results of the low temperature specific heat ( $C$ ) measurements. No ordering have been found down to the lowest temperature of 30 mK. Interestingly,  $C/T$  at zero-magnetic field exhibits a weakly diverging behavior with  $1/T^{0.5}$  temperature dependence. On the other hand, this weakly diverging behavior is suppressed under magnetic field and instead there appears a power law behavior with  $C \sim T^2$ , which is consistent with 2D Dirac fermions. Furthermore, we found a  $T/B$  scaling with a form  $C/B^{0.5} \sim f(T/B)$  for all the data obtained in the temperature and field range below 1 K and 8 T. Interestingly, field induced suppression found in  $1/T_1$  is fully consistent with the  $T/B$  scaling, if we assume that both  $C$  and  $1/T_1$  reflect the density of states arising from the same fermionic excitations. In this presentation, I will further discuss the implication of these observations and possible scenarios for the QSL behaviors. This work has been done in collaboration with Tomohiro Takayama, Kentaro Kitagawa, Riku Takano, Robert Dinnebier, George Jackeli and Hidenori Takagi.

[1] A. Kitaev, Ann. Phys. (N.Y.) 321, 2 (2006).

[2] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009).

[3] Y. Singh and P. Gegenwart, Phys. Rev. B 82, 064412 (2010).

[4] Y. Singh, S. Manni, J. Reuther, T. Berlijn, T. Thomale, W. Ku, S. Trebst and P. Gegenwart, Phys. Rev. Lett. 108, 127203 (2012).

[5] T. Takayama, A. Kato, R. Dinnebier, J. Nuss, H. Kono, L. S. Veiga, G. Fabbri, D. Haskel and H. Takagi, Phys. Rev. Lett. 114, 077202 (2015).



[6] K. Kitagawa, T. Takayama, Y. Matsumoto, A. Kato, R. Takano, Y. Kishimoto, R. Dinnebier, G. Jackeli and H. Takagi, *preprint* (2017).  
Y.Matsumoto@fkf.mpg.de

標題：物質・物性セミナー：Quasi-two dimensional (q2D) organic Mott insulators as seen by inelastic light scattering: from spin liquid to dipole liquid

日時：2017年10月2日(月) 午前11時～午後0時

場所：物性研究所本館6階 第5セミナー室 (A615)

講師：Prof. Natalia Drichko

所属：Department of Physics and Astronomy, Johns Hopkins University

要旨：

Mott insulators are commonly pictured with electrons completely localized on lattice sites. Their low-energy physics involves spins only. In addition, it was shown theoretically that new charge degrees of freedom can emerge in molecule-based Mott insulators as electrons occupy extended molecular orbitals, and can result in a quantum dipole liquid state. We probe few BEDT-TTF-based 2D Mott insulators using Raman scattering technique. We identify magnetic excitation in an antiferromagnetic compound  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Cl and a spin liquid candidate  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub>. We show that their spectrum of excitations is very different from that of a new triangular lattice Mott insulator  $\kappa$ -(BEDT-TTF)<sub>2</sub>Hg(SCN)<sub>2</sub>Br. Our data demonstrate an existence of quantum dipole liquid in this compound. Here, when in the Mott insulating state electrons localize on dimer (BEDT-TTF)<sub>2</sub>lattice sites, they form electric dipoles which do not order at low temperatures. We experimentally detect charge fluctuation with frequency of about 50 cm<sup>-1</sup> using Raman spectra of vibrations of BEDT-TTF molecule. In addition, in the low frequency Raman scattering response we detect a collective mode at about 50 cm<sup>-1</sup> due to respective dipole fluctuations. Heat capacity of  $\kappa$ -(BEDT-TTF)<sub>2</sub>Hg(SCN)<sub>2</sub>Br demonstrates a linear term at low temperatures, supporting a scenario where the composite spin and electric dipole degrees of freedom remain fluctuating down to the lowest temperatures.

標題：理論セミナー：Anomaly Manifestation of Lieb-Schultz-Mattis Theorem and Topological Phases

日時：2017年10月6日(金) 午後4時～午後5時

場所：物性研究所本館6階 第5セミナー室 (A615)

講師：Chang-Tse Hsieh

所属：Kavli IPMU / ISSP

要旨：

The Lieb-Schultz-Mattis (LSM) theorem dictates that any one-dimensional electronic lattice system cannot be a trivial symmetric insulator if the filling per unit cell is not integral and if the lattice translation symmetry and particle number conservation are strictly imposed. In this talk, I will make a comparison between such one-dimensional metallic (gapless) states enforced by the LSM theorem and the boundary gapless states of one-higher dimensional symmetry-protected topological (SPT) phases, from the perspective of quantum anomalies. These two kinds of systems are the rare circumstances where the emergent structures of many-body systems are largely constrained by microscopic kinematic data such as symmetries and spatial dimensions. While at low-energy they are both described by the same effective field theory with the same effective symmetry realizations on low-energy modes, wherein non-site lattice translation symmetry is encoded as if it is a local symmetry, the anomalies of the symmetry in the low-energy theory play different roles in these two systems. In particular, as I will show, the usual chiral anomaly is equivalent to the LSM theorem, whereas there is another anomaly which is not related to the LSM theorem but

intrinsic to the SPT states. As an application, the conventional LSM theorem is extended to multiple-charge multiple-species problems, and several exotic symmetric insulators are constructed.

Reference:

G. Y. Cho, C.-T. Hsieh, and S. Ryu, arXiv:1705.03892 (2017).

(The first two authors contributed equally to the work.)

**標題：極限コヒーレント光科学セミナー：光励起した超伝導体  $\text{La}_{1.85}\text{Sr}_{0.15}\text{Cu}_2\text{O}_4$  における非平衡ジョセフソンプラズマ共鳴**

**日時：2017年10月16日(月) 午前10時～**

**場所：物性研究所本館6階 第一会議室 (A636)**

**講師：松永 隆佑**

**所属：東京大学物性研究所**

**要旨：**

パルスレーザーを用いて物質を超高速に光操作する研究が盛んに行われている中で、近年特に大きなインパクトをもたらした研究の一つが  $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$  で報告された「光誘起室温超伝導」である。他にもいくつかの銅酸化物で類似の現象が観測され[1]、その解釈について盛んに議論が行われている。この一連の実験が光誘起超伝導と解釈されたのは、ジョセフソンプラズマ共鳴(JPR)と呼ばれる光学応答が、光励起後の過渡反射スペクトルに現れたことに起因する。銅酸化物超伝導体は一般に、伝導性の高い  $\text{CuO}_2$  面が絶縁層を挟んで  $c$  軸方向に連なった積層構造を持ち、転移温度以下では  $\text{CuO}_2$  面内の2次元超伝導が天然のジョセフソン接合によって  $c$  軸方向に繋がることでバルク全体として超伝導を示す。この  $c$  軸方向の伝導によるプラズマ端が JPR としてテラヘルツ帯反射率に現れるため、テラヘルツパルスプローブとした時間分解測定が非平衡超伝導研究において重要な役割を果たしている。

これまでの実験は、擬ギャップの現れるアンダードープ領域や、超伝導とストライプ秩序が拮抗する物質など、基底状態の詳細が未だ明らかにされていない系を非平衡にして現れる JPR を議論しているため、解釈が極めて難しい。このような複雑な系について議論する前に、まず典型的な JPR を示す銅酸化物超伝導体を光励起した時に JPR がどう変化するかを明らかにすることが必要である。我々は最適ドープ  $\text{La}_{1.85}\text{Sr}_{0.15}\text{Cu}_2\text{O}_4$  に光励起を行い、平衡下とは異なる JPR が現れる特異な準安定相が出現することを発見した[2]。銅酸化物超伝導の非平衡下の振る舞いに新たな解釈を与えるこの実験結果について議論したい。

[1] For a review, see *e.g.*, D. Nicoletti and A. Cavalleri, *Adv. Opt. Photon.* 8, 401 (2016).

[2] K. Tomari, R. Matsunaga, R. Shimano *et al.*, in preparation.

**標題：物質・物性セミナー：Self-assembled bilayer molecular metals  $(\text{CNB-EDT-TTF})_4\text{X}$ ; The role of C-N…H interactions in a new prototype of 2D Molecular Conductors**

**日時：2017年10月18日(水) 午後3時～午後4時**

**場所：物性研究所本館6階 第5セミナー室 (A615)**

**講師：Prof. Manuel Almeida**

**所属：Instituto Superior Técnico, University of Lisbon**

**要旨：**

The electron donor BEDT-TTF and related symmetrical derivatives have been at the origin of a large number of 2D electronic systems presenting a large diversity of ground states that have been intensively studied during the last years.

In this presentation it will be shown how dissymmetrical ET derivatives like cyanobenzene-ethylenedithio-tetrathiafulvalene (CNB-EDT-TTF), thanks to a combination of C-N…H hydrogen bond assisted dimeric interactions



can be at the origin of a new type of 2D systems, (CNB-EDT-TTF)<sub>4</sub>X, (X= ClO<sub>4</sub><sup>-</sup>, PF<sub>6</sub><sup>-</sup>, I<sub>3</sub><sup>-</sup>, ...) which are characterized by a unique bilayer structure of the donors.

This novel type of salts exhibit 2D metallic properties with special characteristics derived both from the unusual stoichiometry and the weak interaction between paired layers. These properties are related to a high band filling, large electronic effective masses and quasi degenerated 2D Fermi surfaces, as predicted by band structure calculations and in agreement with electron transport measurements in single crystals. Depending on the donor packing pattern some of these 2D metals can present superconductivity at temperatures close to 3K.

The formation of the bilayers by self-assembly is however critically dependent on the counter anions and growth conditions. The rich variety of polymorphism and physical properties that has been recently observed in these (CNB-EDT-TTF)<sub>4</sub>X salts will be also presented in detail.

標題：理論セミナー：Dynamics of confined membranes

日時：2017年10月20日(金) 午後4時～午後5時

場所：物性研究所本館6階 第5セミナー室 (A615)

講師：Olivier Pierre-Louis

所属：CNRS-ILM, Universite Lyon-1

要旨：

Bilayer lipid membranes are abundant in biological systems. They are found in cell membranes, skin, pupils, articulations and pulmonary organs. In biological environments, these membranes are often confined by other membranes or by various substrates. We have investigated the role of confinement on the dynamics of lipid membranes. We first derive a lubrication model for an inextensible bilayer lipid membrane confined between two parallel and flat attractive walls. The resulting model shares similarity the Swift-Hohenberg equation, and with standard coarsening models such as the time-dependent Ginzburg-Landau equation or the Cahn-Hilliard equation. However, our model exhibits a specific behavior controlled by the fixed total quantity of lipids in the system, which imposes a constant total membrane area.

We find that membranes with smaller intrinsic areas form frozen finite-size flat adhesion domains, while membranes with a larger intrinsic area form a frozen labyrinthine wrinkle phase. For intermediate areas, coarsening is found, i.e. an endless increase of the size of adhesion domains. This coarsening behavior is associated to a coexistence between flat adhesion domains and wrinkle domains.

標題：ナノサイエンスセミナー：Spin-polarized scanning tunneling microscopy with quantitative insights into magnetic probes

日時：2017年10月30日(月) 午後1時30分～

場所：物性研究所本館6階 第2会議室 (A635)

講師：Dr. Soo-hyon Phark

所属：enter for Quantum Nanoscience, Institute for Basic Science and

要旨：

Spin-polarized scanning tunneling microscopy and spectroscopy (spin-STM/S) has been successfully applied to magnetic characterizations of individual nanostructures. Spin-STM/S is often performed in magnetic fields of up to some Tesla, which may strongly influence the tip state. In spite of the pivotal role of the tip, the contribution of the tip in spin-STM/S has rarely been investigated in detail. In this talk, an advanced analysis of spin-STM/S data measured on magnetic nanoislands, which relies on a quantitative magnetic characterization of tips, will be discussed. In-field

spin-STM on Co bilayer nanoisland on Cu(111) has enabled a quantitative determination, and thereby, a categorization of the magnetic states of the tips. The resulting in-depth and conclusive analysis of magnetic characterization of the tip opens new venues for a clear-cut sub-nanometer scale spin ordering and spin-dependent electronic structure of the non-collinear magnetic state in bilayer high Fe nanoislands on Cu(111).

This work has been performed in collaboration with Dirk Sander, Max-Planck-Institute of Microstructure Physics, Halle, Germany.

References:

- [1] Rodary, Wedekind, Oka, Sander, Kirschner, Appl. Phys. Lett. 95, 152513 (2009).
- [2] Oka, Ignatiev, Wedekind, Rodary, Niebergall, Stepanyuk, Sander, Kirschner, Science 327, 843 (2010).
- [3] Corbetta, Ouazi, Borme, Nahas, Donati, Oka, Wedekind, Sander, Kirschner, Jpn. J. Appl. Phys. 51, 208 (2012).
- [4] Phark, Fischer, Corbetta, Sander, Kirschner, Appl. Phys. Lett. 103, 032407 (2013).
- [5] Nagai, Hata, Oka, Sander, Kirschner, Appl. Phys. Exp. 7, 025204 (2014).
- [6] Sander, Phark, Corbetta, Fischer, Oka, Kirschner, J. Phys.: Condens. Matter 26, 394008 (2014).
- [7] Phark, Fischer, Corbetta, Sander, Nakamura, Kirschner, Nat. Commun. 5, 5183 (2014).
- [8] Fischer, Sandratskii, Phark, Ouazi, Pasa, Sander, Parkin, Nat. Commun. 7, 13000 (2016).
- [9] Phark, Sander, Nano Convergence 4, 8 (2017).

標題：理論インフォーマルセミナー：Spin Transitions in Spiro-Biphenalenyl-based radicals: Identification of the driving forces and the origin of bistability

日時：2017年10月31日(火) 午後1時～午後2時

場所：物性研究所本館6階 第5セミナー室 (A615)

講師：Prof. Jordi Ribas

所属：Materials Science and Physical Chemistry Department, Universitat de Barcelona

要旨：

Spiro-biphenalenyl (SBP) boron radicals constitute an important family of molecules for the preparation of functional organic materials. The building blocks of several SBP-based crystals are  $\pi$ -dimers of these radicals, in which two phenalenyl (PLY) rings face each other and the other two PLYs point away from the superimposed PLYs. The dimers of ethyl-substituted-SBP and butyl-substituted-SBP undergo a spin transition that results in changes in the magnetic, optical and conducting properties of the material. The spin transition of ethyl-SBP occurs at around 140 K, while the spin transition of butyl-SBP occurs with a hysteretic loop 25 K wide centered at 335 K. In this talk, the results of a computational study aimed at identifying the driving forces of these spin transitions will be presented. The origin of the hysteresis in the phase transition of butyl-SBP will be also disclosed. In particular, it will be shown that electrostatic interactions between radicals play a key role in enabling the spin transitions and that the bistability of butyl-SBP originates in the coupling between the spin transition of its  $\pi$ -dimers and the conformational switch of its butyl chains.



標題：中性子セミナー：Critical dynamics of quantum magnets observed by neutron scattering

日時：2017年11月1日(水) 午後3時～午後4時

場所：物性研究所本館6階 第5セミナー室 (A615)

講師：Dr. Kirill Povarov

所属：スイス連邦工科大学チューリッヒ校

要旨：

Much of interest in quantum magnetic systems is driven by the fact that they serve as excellent realization of quantum critical phenomena. In these situations the finite temperature properties of the materials are defined by the quantum-disordered ground state. Often this concerns not just the thermodynamic properties, but also the details of the excitation spectra [1], which can be directly probed by inelastic neutron scattering. Despite quantum critical dynamics in 1D magnets is rather ubiquitous and has many faces, experimentally observing it is challenging and requires a careful choice of the model material and the measurement parameters. Nonetheless, today's progress in sample synthesis and neutron instrumentation allows to verify many of the long-standing theoretical predictions.

The recent achievements include the “tunable” Tomonaga-Luttinger spin liquids (TLSL) in magnetized  $S=1/2$  spin chains [2] and ladders [3]. In these systems the interactions between the effective fermionic quasiparticles vary as a function of external field [4], and sometimes can even be made attractive instead of a conventional repulsion. In addition to extended quantum critical phases such as TLSL, quantum critical dynamics can be also observed at isolated quantum critical points. For instance, “Ising model in transverse field” -type critical dynamics can be found in a dimerized  $S=1$  chain [5]. The most recent example are the excitations at the saturation field of a quantum spin chain, representing  $z=2$  critical point in one dimension [6]. Inherent to this QCP is the parameterless scaling, known as “zero-scale universality” [7], which, however, is found to be obscured at elevated temperatures.

[1] M. Vojta, Rep. Prog. Phys. 66, 2069 (2003).

[2] M. Haelg *et al.*, Phys. Rev. B 92, 104416 (2015).

[3] K. Povarov *et al.*, Phys. Rev. B 91, 020406 (2015).

[4] T. Giamarchi, *Quantum physics in one dimension* (Oxford University Press, 2003).

[5] M. Haelg *et al.*, Phys. Rev. B 92, 014412 (2015).

[6] D. Blosser *et al.*, arXiv:1707.05243, accepted for Phys. Rev. B

[7] S. Sachdev *et al.*, Phys. Rev. B 50, 258 (1994).

標題：量子物質セミナー：Unveiling the Ground State Properties of the  $S=1/2$  Kagome Heisenberg Antiferromagnet  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$  via Single Crystal NMR

日時：2017年11月6日(月) 午後4時～午後5時

場所：物性研究所本館6階 第5セミナー室 (A615)

講師：Dr. Mingxuan Fu

所属：Department of Physics, University of Toronto

要旨：

The experimental quest for a quantum spin-liquid state (QSL) in frustrated magnetic systems serves fundamental scientific interests, as this intriguing quantum phase provides a fascinating platform for discovering exotic collective phenomena. The  $S=1/2$  kagome Heisenberg antiferromagnet  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$  (herbertsmithite) is one of the leading contenders for an experimental realization of a QSL; in particular, the discovery of a continuum of spinon excitations using inelastic neutron scattering [1] has stimulated intense research into its physical properties. However, the nature of the paramagnetic ground state in this material remains highly debated, primarily owing to the difficulty in revealing

the intrinsic magnetic behaviour of the kagome lattice from defect contributions.

We will discuss our single crystal NMR measurements to probe the local spin susceptibility, low-frequency spin fluctuations, and the effects of defect  $\text{Cu}^{2+}$  spins occupying the  $\text{Zn}^{2+}$  sites. Most importantly, we demonstrate that the low-temperature behaviour of the intrinsic spin susceptibility provides direct evidence for a QSL state with a small energy gap in  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$  [2].

[1] T. H. Han, J. S. Helton, S. Chu, D. G. Nocera, J. A. Rodriguez-Rivera, C. Broholm and Y. S. Lee, *Nature* 492, 406 (2012).

[2] M. Fu, T. Imai, T. H. Han and Y. S. Lee, *Science* 350, 655 (2015).

**標題：セミナー：熱・スピン相互変換**

**日時：2017年11月10日(金) 午後4時～午後5時**

**場所：物性研究所本館6階 第5セミナー室 (A615)**

**講師：大沼 悠一**

**所属：日本原子力研究開発機構**

**要旨：**

電子のスピン自由度の流れであるスピン流は、電流を伴わないため、エネルギー損失を抑えた情報伝達を可能にすると期待されている[1]。スピン流を生成する手法の一つとしてスピンゼーバック効果が知られている[2-4]。磁性体と金属の接合系において、熱からスピン流が生成される。生成スピン流は金属に注入され、スピン軌道相互作用を起源とするスピンホール効果[1]を通して電流に変換される。スピンゼーバック効果が磁性絶縁体であっても発現することから、スピン流を介した新しい熱発電機構として注目を集めている。

スピンゼーバック効果に対して、その逆効果であるスピンペルチェ効果、つまりスピン流による熱流生成現象が近年報告された[5, 6]。磁性体と金属の接合系において金属に電流を流すと、スピンホール効果によって電流がスピン流に変換され、磁性体に注入される。この時、同時に熱流が生成され磁性体に注入される。実際に、金属と磁性絶縁体の界面において発熱と吸熱が同時に観測された[6]。

本講演では、非平衡グリーン関数法を用いて構築した、スピンゼーバック効果とスピンペルチェ効果を統一的に記述する理論を説明し[7]、熱とスピンの相互変換現象の微視的機構を明らかにする。

[1] S. Maekawa, S. O. Valenzuela, E. Saitoh, and T. Kimura, ed., “Spin Current”, Oxford, 2012.

[2] K. Uchida et al., *Nature (London)* 455, 778 (2008).

[3] K. Uchida et al., *Nat. Mater.* 9, 894 (2010).

[4] C. M. Jaworski et al., *Nat. Mater.* 9, 898 (2010).

[5] J. Flipse et al., *Phys. Rev. Lett.*, 113, 027601 (2014).

[6] S. Daimon et al., *Nat. Commun.* 7, 13754 (2016).

[7] Y. Ohnuma et al., *Phys. Rev. B* 96, 134412 (2017).





標題：量子物質セミナー：Chiral liquid phase of simple quantum magnets

日時：2017年11月20日(月) 午後1時30分～午後2時30分

場所：物性研究所本館6階 第2セミナー室 (A612)

講師：Prof. Oleg Starykh

所属：Department of Physics and Astronomy, University of Utah

要旨：

We study a  $T = 0$  quantum phase transition between a quantum paramagnetic state and a magnetically ordered state for a spin  $S = 1$  XXZ Heisenberg antiferromagnet on a two-dimensional triangular lattice. The transition is induced by an easy plane single-ion anisotropy  $D$ . At the mean field level, the system undergoes a direct transition at a critical  $D = D_c$  between a paramagnetic state at  $D > D_c$  and an ordered state with broken  $U(1)$  symmetry at  $D < D_c$ . We show that beyond mean-field the phase diagram is very different and includes an intermediate chiral liquid phase. Specifically, we find that the Ising ( $J_z$ ) component of the Heisenberg exchange creates an attraction between magnons in the paramagnetic phase and binds magnons into a two-particle bound state. This two-magnon bound state condenses at  $D > D_c$ , pre-empting single particle condensation, and gives rise to a chiral liquid phase which spontaneously breaks spatial inversion symmetry, but leaves the spin-rotational and time-reversal symmetries intact. The chiral liquid phase is characterized by a finite vector chirality without long range dipolar magnetic order. We corroborate our analytic treatment with a numerical analysis and show evidence of the chiral phase by means of the density matrix renormalization group calculations.

標題：理論セミナー：Recent Progress in a Calculation Method of Quasiparticle Spectra

日時：2017年12月1日(金) 午後4時～午後5時

場所：物性研究所本館6階 第5セミナー室 (A615)

講師：大野 かおる

所属：横浜国立大学大学院工学研究院

要旨：

Photoelectron spectra represent the total energy difference between the  $N$ -electron system and the  $(N \pm 1)$ -electron system, which give the basic idea of the quasiparticle (QP) energies.

Very recently, we found that the rigorous formulation involving the QP energies, the QP wave functions, and the QP equation can be applied not only to the  $N$ -electron ground state but also to any  $M$ -electron excited eigenstate [1]. Focusing on this topic, I will explain our recent achievement of the self-consistent  $GW\Gamma$  calculation [2], the GW without Bethe-Salpeter equation method for photoabsorption spectra [3], and the TDGW method for excited state dynamics simulations [4]. These calculations were carried out by using the all-electron mixed basis approach (program name TOMBO), which uses both numerical atomic orbitals and plane waves [5].

[1] K. Ohno, S. Ono, and T. Isobe, *J. Chem. Phys.* 146, 084108 (2017).

[2] R. Kuwahara, Y. Noguchi, and K. Ohno, *Phys. Rev. B* 94, 121116(R) (2016).

[3] T. Isobe, R. Kuwahara, and K. Ohno, to be submitted.

[4] T. N. Pham, S. Ono, and K. Ohno, *J. Chem. Phys.* 144, 144309 (2016).

[5] S. Ono, Y. Noguchi, R. Sahara, Y. Kawazoe, and K. Ohno, *Comp. Phys. Comm* 189, 20 (2015).

**標題：極限コヒーレント光科学セミナー：水と氷のネットワーク構造と物性**

**日時：2017年12月12日(火) 午前10時～午後0時**

**場所：物性研究所本館6階 第一会議室 (A636)**

**講師：松本 正和**

**所属：岡山大学異分野基礎科学研究所**

**要旨：**

水に物質を溶かすと何が起るか。それに答えるためには、水そのものの性質をよく知る必要がある。水は塩も砂糖も油も気体もプロトンもタンパク質も溶かしてしまうが、単にエントロピーをかせいであるだけでなく、溶質の種類に合わせて、水自体が構造を変えたり、溶質と一体化してしまったりする。そのため、溶質分子の間に奇妙な引力が働いたり、違う種類の物質を同時に溶かすと意外なことが起きたりする。さらに、物質を溶かすと、氷の結晶構造が大幅に変わり凝固点が上昇することもある。溶媒と溶質を地(背景)と図(主体)として分けてしまえない、これらのさまざまな水和現象を理解する基礎として、水の作る多様な構造と物性を紹介したい。

[1] Matsui, T., Hirata, M., Yagasaki, T., Matsumoto, M. & Tanaka, H. *J. Chem. Phys.* 147, 091101 (2017).

[2] Matsumoto, M., Yagasaki, T. & Tanaka, H. *Phys. Rev. Lett.* 115, 197801 (2015).

[3] Yagasaki, T., Matsumoto, M. & Tanaka, H. *Phys. Rev. E* 89, 020301 (2014).

[4] M. Matsumoto and H. Tanaka, *J. Phys. Chem. B*, 115, 8257 (2011).

[5] M. Matsumoto, A. Baba, and I. Ohmine, *J. Chem. Phys.* 127, 134504 (2007).

**標題：理論セミナー：コニカルらせん磁性体におけるマルチフェロイックドメイン制御**

**日時：2017年12月15日(金) 午後4時～午後5時**

**場所：物性研究所本館6階 第5セミナー室 (A615)**

**講師：木村 剛**

**所属：東京大学新領域創成科学研究科**

**要旨：**

コニカルらせん磁気構造を持つマルチフェロイクスにおいては、ときに自発分極と自発磁化が共存し、磁化の反転に伴って自発分極が反転するといった稀有な電気磁気結合が発現する。本講演では、コニカルらせん磁気構造を示すマルチフェロイクスとして六方晶フェライト  $\text{Ba}_{1.3}\text{Sr}_{0.7}\text{CoZnFe}_{11}\text{AlO}_{22}$ 、オリビン型 Mn 酸化物  $\text{Mn}_2\text{GeO}_4$  などを取り上げ、円偏光共鳴軟 X 線回折や偏極中性子線回折測定により明らかとなったマルチフェロイックドメインの実空間分布やその外場応答に関する結果を紹介し、コニカルらせん磁性体における多様なドメイン（強磁性・強誘電・磁気らせん・ $180^\circ$  反強磁性ドメイン等）のスイッチに起因する電気磁気結合に関して議論する。本講演の内容は、上田大貴(阪大基礎工)、田中良和(理研 Spring-8 センター)、本田孝志(KEK 物構研)、J.S. White (PSI), M. Kenzelmann (PSI)らとの共同研究によるものである。

[1] H. Ueda, Y. Tanaka, H. Nakajima, S. Mori, K. Ohta, K. Haruki, S. Hirose, Y. Wakabayashi and T. Kimura, *Appl. Phys. Lett.* 109, 182902 (2016).

[2] T. Honda, J. S. White, A. B. Harris, L. C. Chapon, A. Fennell, B. Roessli, O. Zaharko, Y. Murakami, M. Kenzelmann, and T. Kimura, *Nat. Commun.* 8, 15457 (2017).



標題：理論セミナー：Competing orders in Dirac fermions  
日時：2017年12月19日(火) 午前10時30分～午前11時30分  
場所：物性研究所本館6階 第5セミナー室 (A615)  
講師：Toshihiro SATO  
所属：Universität Würzburg  
要旨：

Correlated Dirac systems are currently one of the most active research areas in condensed matter physics. The topic is experimentally relevant in the context of graphene and other Dirac materials, and theoretically relevant because the corresponding low-energy field theories exhibit remarkable topological properties and are closely related to high-energy physics. We will present exact quantum Monte Carlo results for a model of Dirac fermions in 2+1 dimensions with dynamically generated, anti-commuting  $SO(3)$  Néel and  $Z_2$  Kekulé mass terms. We will provide evidence for a direct and continuous transition between the Néel and Kekulé phases. The fermions remain gapped across the transition, and our data support an emergent  $SO(4)$  symmetry unifying the two order parameters. While this phase transition falls outside the Ginzburg-Landau-Wilson paradigm, the emergent  $SO(4)$  invariance permits an interpretation of the transition in terms of deconfined quantum criticality [1].

References:

[1] T. Sato, M. Hohenadler, and F. F. Assaad, Phys. Rev. Lett. 119, 197203 (2017).

標題：理論セミナー：結合クラスター理論に基づいた1電子スペクトル計算  
日時：2017年12月22日(金) 午後4時～午後5時  
場所：物性研究所本館6階 第5セミナー室 (A615)  
講師：松下 雄一郎  
所属：東京大学大学院工学系研究科  
要旨：

密度汎関数理論(DFT)は弱相関物質に対して適用された際に、極めて精度良く電子状態や原子構造を記述することが知られており、解析・予言の様々な面で用いられてきた。しかし、強相関電子系を代表とするいくつかの系においては定性的にも誤った結果を出す事が知られている。一方で、波動関数理論は孤立系(原子・分子系)へと適用され、DFTを超えた高精度計算がなされている。しかし、一般に波動関数理論の下では全エネルギーに対する信頼性の高い計算が可能となる一方で、エネルギー準位(1電子準位)の解析に関しては極めて限定的であった。本研究では、波動関数理論としてcoupled-cluster(CC)理論を採用し、CC理論の下で1粒子グリーン関数を構築する事により1電子スペクトルを計算し、厳密解と比較を行った。その結果、準粒子スペクトルを極めて良い精度で再現すること、さらにはサテライトピーク(共鳴準位)に関しても再現される事を見出した。本発表では、孤立原子を中心に結果を紹介する。