# 物性研究所セミナー

標題:Functional-renormalization-group approach to classical liquids

日時: 2023 年 3 月 15 日(水) 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)とオンライン(Zoom)のハイブリッド形式

講師:横田 猛

所属:理化学研究所 数理創造プログラム

要旨:

Accurate and efficient ways to analyze classical liquids are desired in various contexts including chemical reactions. Traditional approaches include the renormalization-group (RG) methods such as the hierarchical reference theory. However, these traditional approaches rely on the knowledge of hard-core reference systems to include the effect of short-range repulsion. Recently, we have developed an RG approach that does not rely on a hard-core reference system [1]. We have introduced the functional RG to rigorously describe the RG flow and the cavity distribution functions to treat short-range repulsion. In this talk, I will present the formulation and numerical demonstrations in a one-dimensional solvable model, where our approach shows better accuracy than the conventional integral-equation methods such as the hypernetted chain and the Percus-Yevick equation.

[1] T. Yokota, J. Haruyama, O. Sugino, Phys. Rev. E 104, 014124 (2021).

標題:空間反転対称性の破れた有機・無機ハイブリッドペロブスカイト系化合物における光 - スピン物性

日時: 2023年3月17日(金)午前11時~午後0時

場所:Online

講師:谷口 耕治 教授

所属:東京工業大学理学院

要旨:

有機・無機ハイブリッドペロブスカイト(OIHP)系化合物は、優れた太陽電池材料としての特性を示すことなどから、その光物性が近年注目を集めている。OIHP 系化合物は、無機骨格に磁性元素や重元素を組み込むことが可能であり、優れた光物性をスピン物性と結合させる舞台として興味深い系である。最近、我々のグループでは、OIHP 系化合物へのキラリティの導入を介して、空間反転対称性の破れを制御した物質開発を行ってきた。本セミナーでは、新規に開発した空間反転対称性の破れた系において、発現が確認された非反転対称性誘起の光 - スピン結合物性として、非相反的方向二色性と非線形光伝導現象に関して発表した。

標題: Spin-derived electric polarization and chirality density inherent in localized electron orbitals

日時: 2023年3月27日(月)午後4時~午後5時

場所:Online 講師:星野 晋太郎 所属:埼玉大学

要旨:

In solid state physics, any phase transition is commonly observed as a change in the microscopic distribution of charge, spin, or current. However, there is an exotic order parameter inherent in the localized electron orbitals that

 cannot be primarily captured by these three fundamental quantities.

This order parameter is described as the electric toroidal multipoles connecting different total angular momenta under the spin-orbit coupling. The corresponding microscopic physical quantity is the spin current tensor on an atomic scale, which induces spin-derived electric polarization aligned circularly and the chirality density derived from the Dirac equation [1].

We also derive the equation of continuity for chirality density and discuss its relation to chiral anomaly and optical chirality. These findings link microscopic spin currents and chirality in the Dirac theory to the concept of multipoles and provide a new perspective for quantum states of matter.

This work has been done in collaboration with H. Ikeda and M.-T. Suzuki.

[1] S. Hoshino, M.-T. Suzuki, H. Ikeda, arXiv:2210.02148 (2022).

標題:動的平均場法による多極子感受率と多極子相互作用の導出

日時: 2023年3月28日(火)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) 及び Online

講師:大槻 純也

所属:岡山大学異分野基礎科学研究所

要旨:

近年、動的平均場近似によって多体効果を考慮した強相関化合物の電子状態計算法、いわゆる LDA+DMFT 法(または DFT+DMFT 法)が急速な発展を見せている。この方法を用いることで、3d 軌道や4f 軌道などの局在性の強い軌道を含む電子状態を記述することが可能となる。それにより、電子の局在状態における磁性(多極子秩序)や遍歴状態における磁性と超伝導も統一した近似で議論できるようになると期待される。

我々は、この方法論により多極子感受率を評価することで、強相関化合物の多極子相転移の予測を目指して研究を行っている。講演では特に、この研究に関する下記の2つの進展について紹介した。

- ・強相関極限で厳密なベーテ・サルペータ方程式の近似公式 [1]
- ・4f 電子系の多極子秩序の典型物質である CeB6 への応用 [2]

ひとつめは、多極子感受率の計算でネックとなる軌道数の 4 乗に比例した成分数を持つベーテ・サルペータ方程式の扱いを簡略化するものである。ふたつめでは、第一原理計算と組み合わせた計算により、CeB6 における反強四極子秩序(II 相)の相転移温度が適度な精度で見積もられた例を紹介した。

- [1] J. Otsuki, K. Yoshimi, H. Shinaoka, Y. Nomura, Phys. Rev. B 99, 165134 (2019).
- [2] J. Otsuki, K. Yoshimi, H. Shinaoka, H. O. Jeschke: arXiv:2209.10429.

標題: Quantum Geometric Light-Matter Interactions and Optical Control in Correlated and Open Quantum Systems

日時: 2023 年 3 月 31 日(金) 午前 10 時~午前 11 時

場所:Online

講師: Martin Claassen

所属: The University of Pennsylvania

# 要旨:

Irradiation with light provides a powerful tool to interrogate, control or induce new quantum states of matter out of equilibrium, however a microscopic understanding of dynamics and light-matter coupling in solids remains a profound challenge. This talk will discuss three aspects for steering and probing correlated topological matter, dissipative electron systems and superconductors with light. I will show that THz radiation can grant a new quantum-geometric handle to steer correlated quantum materials such as magic-angle twisted bilayer graphene, whereby light dynamically dresses the Wannier functions of interacting electrons which govern the low-energy dynamics. I will then discuss how light can couple to open electronic quantum systems interacting with Markovian reservoirs, to permit a spectroscopic probe of dissipation-engineered Lindbladian band structures and exceptional points in low-dimensional systems. Finally, I will argue that dynamical symmetry breaking with tailored light pulses can explore metastable phases in superconductors with competing instabilities, as a route to stabilize elusive triplet paired states.

標題: π共役分子の一次元配列を基点とした未来材料探索

日時: 2023 年 4 月 13 日(木) 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:宮島 大吾

所属:凝縮系物性研究部門、JST さきがけ

#### 要旨:

有機材料(=分子性材料)の物性は構成する分子の構造と集合様式によって決まる。計算科学の発展により分子単体の物 性はかなり正確に予測できるようになりつつあるが、分子の集合構造の予測は未だ困難である。 集合構造を制御するツ ールとして、我々はこれまでアミド基の水素結合を利用し超分子ポリマーやカラムナー液晶の研究を行ってきた。重合様 式・強誘電性など、アミド基の特性を生かした種々の物性・機能を報告してきた1-3)。さらに近年超分子重合と自己複製 反応を組み合わせた固相超分子重合の系も見出した 4)。しかしながら、アミド基のような水素結合ユニットや Metal Organic Framework (MOF)に用いられる配位結合を用いることが必ずしも物性面において良い結果をもたらすわけでは ない。本セミナーではアミド基など強い分子間相互作用ユニットを用いないπ共役分子の配列制御と、その分子配列戦略 に基づく未来材料探索について紹介した5-8)。

- 1) Science, 336, 209-213, 2012.
- 2) Science, 347, 6222, 646-651, 2015.
- 3) Nature Chem. 9, 1133-1139, 2017.
- 4) Nat. Mater. 21, 253-261, 2022.
- 5) J. Am. Chem. Soc., 142, 3326-3330, 2020.
- 6) Angew. Chem. Int. Ed., 60, 16377-16381, 2021.
- 7) Angew. Chem. Int. Ed., 60, 3261-3267, 2021.
- 8) Nature, 609, 502-506, 2022.

標題: Microscopic theory of spin Hall magnetoresistance

日時:2023年4月14日(金)午後4時~午後5時

場所:物性研究所本館 大講義室 (A632) /Online

講師:加藤 岳生

所属:東京大学物性研究所

要旨:

Magnetoresistance has been one of the important phenomena in spintronics for a long time. Recently, a novel type of magnetoresistance called spin Hall magnetoresistance (SMR) has been observed in a bilayer system composed of a normal metal and a ferromagnetic insulator. While its qualitative behavior has been explained well by the semiclassical theory based on a mixing conductance [1], this theory could not describe temperature dependence of the SMR. In this talk, I present a microscopic theory [2,3] for SMR by formulating a spin conductance in terms of spin susceptibilities. We reveal that SMR is composed of static and dynamic parts; The static part originates from spin flip caused by an interfacial exchange coupling. On the other hand, the dynamic part, which is induced by the creation or annihilation of magnons, has an opposite sign from the static part. I also present the temperature dependence of SMR derived by our theory using the spin-wave approximation [2] and a quantum Monte Carlo simulation [3].

[1] Y. T. Chen, et al., Phys. Rev. B 87, 144411 (2013).

[2] T. Kato, Y. Ohnuma, and M. Matsuo, Phys. Rev. B 102, 094437 (2020).

[3] T. Ishikawa, M. Matsuo, and T. Kato, Phys. Rev. B 107, 054426 (2023).

標題:Higher-group symmetry of topological order and stabilizer codes

日時:2023年4月18日(火)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:小林 良平

所属:University of Maryland

要旨:

Topologically ordered phases can host interesting classes of non-trivial topological defects of varying codimensions. Among the topological defects, the invertible defects form an algebraic structure called higher-group. In this talk we explain how the higher-group structure of invertible global symmetry emerges in discrete gauge theory of generic dimensions, and show various examples of the higher-group symmetry in topological order mainly focusing on (3+1)-dimensional stabilizer codes. The emergent global symmetry of a stabilizer model is understood as a logical gate acting on the logical qubits. We explain that the higher-group structure of global symmetry in general leads to non-Pauli logical gate realized by the action of emergent global symmetry, e.g., Control-Z logical gate of (3+1)-dimensional Z2 toric code.

標題: Error-correction assisted measurement of Membrane operators in Ultracold Atom simulators

日時:2023年4月27日(木)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: Gil Young Cho

所属: Pohang University of Science and Technology

要旨:

Exotic quantum many-body state, such as Haldane and spin liquid phases, can exhibit intriguing features like fractional excitations and non-abelian statistics, and provide new understandings of quantum entanglement in many-body systems. They are often indistinguishable from trivial states from the perspective of Landau's symmetry breaking paradigm and are classified by non-local correlators. However, the characterization of these phases is experimentally challenging since the non-local correlators are sensitive to incoherent errors like atom losses, which suppress its signals exponentially. Additionally, there has not been much progress in developing protocols, which systematically identify and mitigate the incoherent errors in the analog quantum simulator. Here, we address these challenges by developing an error correction protocol for large-scale neutral atom quantum simulators using optical lattices, which simulate the strong-correlation physics of the paradigmatic two-dimensional Bose-Hubbard model. We develop and apply a new error correction approach based on the Ising model, which enables us to identify and remove uncorrelated errors in the quantum simulations. After correcting such incoherent errors, we observe a dramatic improvement of the parity correlator and find the perimeter scaling law in two-dimensional Mott insulators. Furthermore, the error model provides a statistical estimation of number fluctuations, from which we can measure the generalized brane order parameter. Our work provides a promising avenue for investigating and characterizing exotic phases of matters in large-scale quantum simulations.

標題: Exploring Electron Pairing Symmetry in CsV3Sb5-Derived Kagome Superconductors Utilizing Ultrahigh Resolution laser-ARPES

日時: 2023年4月27日(木)午後0時15分~午後1時15分

場所: Online

講師: Yigui Zhong

所属: Okazaki group in LASOR

要旨:

The newly discovered kagome superconductors AV3Sb5 (A=K, Rb, Cs) represent a promising platform for investigating the interplay between band topology, electronic order, and lattice geometry [1, 2]. Despite extensive research efforts on this system, the nature of the superconducting ground state remains elusive and a consensus on the electron pairing symmetry has not been achieved so far. In this talk, I will report our ultrahigh resolution and low-temperature angle-resolved photoemission spectroscopy (ARPES) studies on two exemplary CsV3Sb5-derived kagome superconductors — Cs(V0.93Nb0.07)3Sb5 with the appearance of charge order and Cs(V0.86Ta0.14)3Sb5 without charge order in the normal state [3]. Additionally, I will present our studies of electronic kinks in the band structure [4] and temperature-dependent muon spin relaxation rate, and discuss the possible pairing mechanisms for these kagome superconductors. Overall, our findings contribute to a better understanding of the nature of superconductivity and its intertwined orders in kagome quantum materials.

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# References:

[1] Neupert, T. et al., Nature Physics 18, 137 (2021).

[2] Yin et al., Nature 612, 647-657 (2022).

[3] Zhong, Y. et al., Nature, in press, arXiv:2303.00875.

[4] Zhong. Y. et al., Nat. Commun., in press, arXiv:2207.02407.

標題: Zeros of Green functions in topological insulators – A tool for visualizing topological phases

日時: 2023年5月15日(月)午後1時~午後2時

場所:Online

講師: Takahiro Misawa

所属: ISSP

要旨:

Recently, we have found that the zeros of the diagonal components of the Green functions are useful quantities for detecting a wide range of topological insulators [1]. In particular, we have shown that the zeros of the Green functions traverse the band gap due to band inversions in the topological phases. Utilizing this feature, we can distinguish topological phases by seeing whether the zeros traverse the band gap. For microscopic models of the conventional six classes of topological insulators, we show that the traverses of the zeros universally occur in the topological phases. We also show that higher-order topological insulators, which have recently attracted much attention, can also be detected by the zeros of the Green functions.

Interestingly, the recently rediscovered eigenvector-eigenvalue identity [2], which is a simple but long-time-overlooked mathematical formula in linear algebra, plays an important role in the analysis of the zeros of the Green functions. Furthermore, by using the zeros of the Green function, we find that a conventional antiferromagnetic Mott insulator in  $\kappa$ -(BEDT-TTF)2Cu[N(CN)2]Cl can be regarded as a correlated topological insulator [3].

### References

[1] T. Misawa and Y. Yamaji, Phys. Rev. Research 4, 023177 (2022).

[2] P. Denton, S. Parke, T. Tao, and X. Zhang, Bull. Am. Math. Soc. 59, 31 (2022). The story on the finding of the eigenvector-eigenvalue identity is available at https://www.quantamagazine.org/neutrinos-lead-to-unexpecteddiscovery-in-basic-math-20191113/

[3] T. Misawa and M. Naka, arXiv:2301.04490.

標題: Anomalous spin wave excitations in quantum antiferromagnets CsFeCl3 and RbFeCl3

日時: 2023 年 5 月 17 日(水) 午後 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)及び Zoom(ハイブリッド開催)

講師:林田 翔平

所属: Max-Planck-Institute for Solid State Research

要旨:

The alkali-metal trichloroferrates AFeCl3 (A = Cs and Rb) are prototypical S = 1 triangular quantum antiferromagnets with strong planar magnetic anisotropy [1]. Under the influence of hydrostatic pressure [2] or chemical composition [3], they are known to exhibit quantum phase transitions between gapped quantum-paramagnetic and magnetically ordered states. A combination of quantum criticality and geometrical frustration makes spin dynamics in AFeCl3 complex and intriguing. However, a comprehensive understanding is still lacking. In this talk, I present a detailed quantitative analysis of the spin-wave excitations by neutron scattering technique [2,3] and the extended spin-wave theory (ESWT) [4]. The spin-wave analysis seems to work reasonably well for CsFeCl3, but the ESWT fails already on a quantitative level for RbFeCl3. The most striking finding is that the measured spin-

wave intensity is highly anisotropic in the long-wavelength limit, whereas the ESWT simulation based on short-range interaction alone predicts an isotropic spectrum. We conclude that this discrepancy is attributed to long-range dipolar interactions [5].

#### References

- [1] H. Yoshizawa et al., J. Phys. Soc. Jpn. 49, 144 (1980).
- [2] S. Hayashida et al., Sci. Adv. 5, eaaw5639 (2019).
- [3] S. Hayashida et al., Phys. Rev. B 99, 224420 (2019).
- [4] M. Matsumoto, S. Hayashida, and T. Masuda, J. Phys. Soc. Jpn. 89, 034710 (2020).
- [5] L. Stoppel, S. Hayashida et al., Phys. Rev. B 104, 094422 (2021).

標題: Spin-to-charge conversion with various quantum materials

日時: 2023 年 5 月 22 日(月) 午後 2 時~午後 3 時

場所:物性研究所本館6階 第5セミナー室(A615)

講師: Subhankar Bedanta

所属: National Institute of Science Education and Research (NISER)

# 要旨:

The precession of magnetization in a ferromagnet (FM) can transmit pure spin current into an adjacent heavy metal (HM) via spin pumping. This pure spin current gets converted to charge current due to high spin orbit coupling (SOC) of the HM due to the inverse spin Hall effect (ISHE). I will discuss recent ISHE results on Co2Fe0.4Mn0.6Si/Pt bilayers, where Co2Fe0.4Mn0.6Si is a full Heusler alloy. Damping analysis indicates the presence of significant spin pumping at the interface of Co2Fe0.4Mn0.6Si and Pt [1]. I will also discuss ISHE experiments on some other combinations such as CoFeB/IrO2 and manganite based La0.66Sr0.34MnO3/Pt bilayers. [2-3] Recently AFM materials having high SOC have been found to be a good replacement of HM in spin current based study. We have performed the ISHE study of CoFeB (10 nm)/ AFM (d nm) where we considered various AFM such as Mn2Au, IrMn, Mn3Ga etc. The systematic angle dependent ISHE measurements have been carried out to disentangle the different spin rectification effects viz. anisotropic magnetoresistance and anomalous Hall effect [4 – 6]. Further I will show the ISHE study on topological insulator (TI)/ferromagnetic Bi2Se3/CoFeB films [7,8]. ISHE experiments have also been performed to demonstrate that TIs are potential candidates to replace HM as they possess high spin-orbit coupling.

Acknowledgements: I like to thank my collaborators and funding agencies for their generous support.

- [1] B. B. Singh et al., NPG Asia Materials, 13, 9 (2021).
- [2] B. Sahoo et al. Adv. Quant. Technol. 2021, 2000146 (2021).
- [3] P. Gupta et al., Nanoscale, 13, 2714-2719, (2021).
- [4] B. B. Singh and S. Bedanta, Phys. Rev. Applied 13, 044020 (2020).
- [5] B. B. Singh et al., Phys. Rev. B 102, 174444 (2020).
- [6] K. Roy et al., J. Phys. D Appl. Phys. 54, 425001 (2021).
- [7] B. B. Singh et al., PSS Rapid 2018, 1800492 (2018).
- [8] B. B. Singh et al., ACS Applied Material & Interfaces 12, 53409 (2020).

標題: Drude weights and f-sum rules for linear and nonlinear conductivities

日時: 2023年5月26日(金)午後4時~午後5時

場所:物性研究所本館 第5セミナー室(A615) /Online

講師:押川 正毅 所属:物性研究所

要旨:

Conductivity is one of the most important characteristics of materials. Nonlinear conductivities are of increasing experimental and theoretical interest recently, but the subject is largely open. I will discuss our recent approach to the fundamentals of the nonlinear conductivities. An application of a spatially uniform electric field can be formulated as an insertion of Aharonov-Bohm flux. By considering the energy gain of the system in the two opposite limits of flux insertion — adiabatic and sudden, we can derive the two renowned formulae on linear conductivities: Kohn formula for Drude weights and the f-sum rule, in a unified manner. Furthermore, they can be naturally generalized to all orders of nonlinear conductivities.

The Drude weight obtained from the nonlinear generalization of Kohn formula often turns out to be divergent. We argue that the divergence is due to the order of limits intrinsic to the Kohn formula, in which the adiabatic (zero frequency) limit is taken before the thermodynamic limit.

#### References:

1. Watanabe and M. O., Phys. Rev. B 102, 165137 (2020).

2. Watanabe, Y. Liu, and M. O., J. Stat. Phys. 181, 2050 (2020).

3.Takasan, M.O., and H. Watanabe, Phys. Rev. B 107, 075141 (2023).

標題: Specific Heat of Quantum Materials in high magnetic fields 強磁

日時: 2023年5月26日(金)午前11時~午後0時

場所:Online

講師: Dr. Christophe Marcenat

所属: CEA-Grenoble

要旨:

In the introduction, I will briefly explain recent improvements in the technique of modulation calorimetry which allows ultra high sensitivity and provides a new tool for fermiology and the study of quantum oscillations.

Thereafter I will illustrate these new possibilities in 3 different cases: the (ultra) quantum limit of graphite, the search for chargeless fermions in Kondo insulators, and the exotic superconductivity in UTe2.

標題:マグノン流体における Wiedemann-Franz 則の破れ

日時:2023年6月9日(金)午後4時~午後5時

場所:物性研究所本館 6階 A615号室 及び Online

講師:佐野 涼太郎

所属:京都大学理学研究科

#### 要旨:

量子輸送現象は、基礎・応用両面での重要性から、物性物理学において大きな関心を集めてきた。さらに近年における 実験技術の躍進により、量子輸送の研究はますます加速しつつある。最近実現できるようになった超純良な系では、準粒 子間の強い相互作用によって輸送特性が大きく変えられ、流体力学的な兆候が現れることが報告され始めている。その最 も顕著な例として、金属における流体力学的な電荷輸送が挙げられ、「電子流体力学」と呼ばれる新たな潮流を生み出し てきた[1]。実際、この概念の登場を皮切りに、負の非局所抵抗[2]や Wiedemann-Franz (WF) 則の破れ[3]など様々な非 従来型の輸送現象が明らかにされつつある。

一方で近年、超純良な強磁性絶縁体の実現により、マグノン流体への道もまた開拓され始めている[4]。マグノンは、ジュール熱を伴わないスピンの担い手として注目されており、特に流体力学的なマグノン輸送は電子流体と同様、従来的な自由粒子描像を超えたこれまでにない革新的な機能性を秘めている[5]。しかしながら現時点では、この領域特有の時間および長さスケールに直接アクセスできるプローブがないため、マグノン流体の観測は未だに実現されていない。

そこで本研究では、特に時間スケールに着目することにより、マグノン流体方程式を導出するとともに、スピン伝導度および熱伝導度を考察した[7]。さらに、流体力学領域に特有なスピン流と熱流の緩和機構の違いにより、従来的な輸送領域で成り立つマグノン WF 則[6]が大きく破れることを明らかにした。従って本結果は、マグノンの流体的な振る舞いが実現していることを示唆する重要な証拠となるのみならず、マグノン流体観測に大きく貢献すると期待される。

- [1] J. Crossno, et al., Science 351, 1058 (2016).
- [2] D. Bandurin, et al., Science 351, 1055 (2016).
- [3] J. Gooth, et al., Nat. Comm. 9, 4093 (2018).
- [4] C. Du, et al., Science 357, 195 (2017).
- [5] C. Ulloa, et al., PRL 123, 117203 (2019).
- [6] K. Nakata, et al., PRB 92, 134425 (2015).
- [7] R. Sano and M. Matsuo, PRL 130, 166201 (2023).