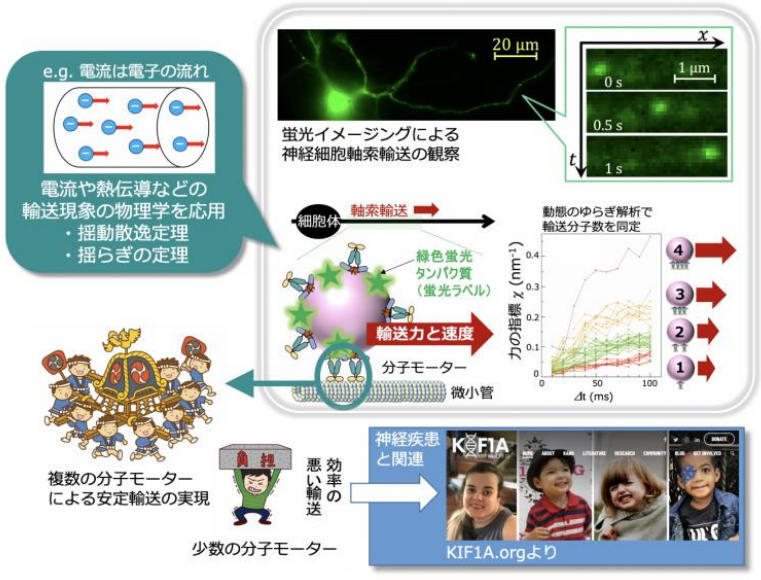
物性研究所セミナー

標題：非平衡統計力学を用いた生体内輸送現象の研究
日時：2022 年 6 月 16 日(木)　午前 10 時～午前 11 時 30 分
場所：Online
講師：林 久美子
所属：東北大学　大学院工学研究科　応用物理学専攻
要旨：

アインシュタイン関係式やグリーン・久保公式に代表される揺動散逸定理（線形応答理論）は、外場の小さい線形応答領域で成立する関係式である。フラストレーションのあるスピングラスや構造ガラス、強い外場で駆動される粒子系では揺動散逸定理の破れが報告されている。揺動散逸定理の破れは生物系でも報告があり、本研究では神経細胞内の軸索輸送という生体内の輸送現象に着目する。

神経細胞は核があり物質合成を行う細胞体とシナプスのある末端領域が長い軸索を介して結合されている。その両末端間の物流を担うのが軸索輸送であり、分子モーター（キネシンとダイニン）が微小管というレールに沿って物質を輸送する。分子モーターは細胞内で、アデノシン三リン酸加水分解で得た化学エネルギーを歩行という力学エネルギーに変換して機能するタンパク質である。神経細胞軸索輸送は蛍光顕微鏡を用いて観察する。本研究では緑色蛍光タンパク質を蛍光ラベルとして用い、輸送動態の非平衡揺らぎ解析のために 10 ms の高速イメージングを行った。

神経細胞内という強い非平衡系では統計物理法則が成り立たず、物性計測が難しくなる。このような状況で、どのように輸送力や輸送速度などの物理パラメータを見積もり、軸索輸送を物理系として理解するかが問題である。また、軸索輸送は神経細胞の物流の要であるため、軸索輸送障害と神経疾患は深い関係がある。本研究では特に KIF1A 関連神経障害としての痙性対麻痺やミトコンドリア病などの疾患メカニズム理解のための取り組みについて話す。物理学、特に非平衡統計力学を医学に役立てる挑戦を紹介した。



標題：Improvement of the Tensor Renormalization Group Methods
日時：2022 年 6 月 17 日(金)　午後４時～午後５時
場所：Online
講師：Dr. Satoshi Morita
所属：ISSP, The University of Tokyo
要旨：

The tensor network (TN) is a powerful tool to calculate and understand strongly correlated many-body problems. The partition function in classical statistical systems can easily be represented as a tensor network. Combining the real-space renormalization group and TNs, the tensor renormalization group method (TRG) provides an efficient contraction scheme for TNs. Information compression based on the singular-value decomposition avoids exponential divergence of a computational cost. In this talk, we will present our recent new ideas in the tensor renormalization group. The first one is a calculation method for higher-order moments of physical quantities such as magnetization [1]. The systematic summation technique provides the recursion formula for coarse-graining tensors including multiple impurities. Our method easily approaches a huge system size which the Monte Carlo method cannot treat. The second one is an efficient algorithm for global optimization technique which improves the accuracy of TRG [2]. By replacing the environment tensor with the corner transfer matrices, we succeed to reduce the order of the computational cost.

[1] Satoshi Morita and Naoki Kawashima, Comput. Phys. Comm. 236, 65–71 (2019).
[2] Satoshi Morita and Naoki Kawashima, Phys. Rev. B 103, 045131 (2021)

標題：Nano Science Seminar: Atomic scale growth and investigation of novel 2D materials
日時：2022 年 6 月 22 日(水)　午後４時～午後５時 30 分
場所：Online
講師：Prof. Matthias Batzill
所属：Dept. Physics, Univ. of South Florida, and ISSP, Univ. Tokyo
要旨：

Modifying bulk surfaces by metal deposition is well established method to create low dimensional materials for fundamental studies of quantum properties. However, the confinement to materials surfaces, makes it challenging to integrate these materials into devices. In contrast to bulk surfaces, van der Waals materials are stable as free-standing 2D sheets in various environments and can be readily manipulated and integrated with other materials. Here we explore if such 2D transition metal dichalcogenides can be modified by metal deposition (similar to bulk surfaces) to create nanostructures with new properties.

2D materials are lacking dangling bonds and thus unlike bulk surfaces, are considered to interact weakly with metal atoms and thus are assumed to favor the agglomeration of atoms into clusters on their surface. Here we show that for some transition metal dichalcogenides (TMDs) this notion of a weak interaction of vapor deposited metals on TMDs is not always true and their 2D-crystal structure can be modified by reaction with vapor deposited metals. We discuss this on the example of two different TMDs, semiconducting Mo-dichalcogenides and semi-metallic PtTe2. For the former we show that Mo-deposition results in the formation of metallic 1D line-defect networks and we discuss the underlying materials physics of their formation [1]. Moreover, the 1D electronic nature of these defects, embedded in the semiconducting host material, is confirmed by angle resolved photoemission spectroscopy that shows signatures of a Tomonaga Luttinger liquid [2]. The modification of MoSe2 can also be expanded to hetero-atoms and these may induce magnetism in the material, forming a diluted ferromagnetic 2D-semiconductor [3]. Finally, for PtTe2 we show

that Pt-deposition converts the 2D-PtTe2 (ditelluride) into metastable 2D-PtTe (monotelluride) [4]. In the monolayer, this enables the construction of a metal/semiconductor junction in 2D materials, whose interface properties can be studied by scanning tunneling spectroscopy.

[1] P.M. Coelho, H.-P. Komsa, H.C. Diaz, Y. Ma, A.V. Krasheninnikov, M. Batzill. Post-Synthesis Modifications of Two-Dimensional MoSe2 or MoTe2 by Incorporation of Excess Metal Atoms into the Crystal Structure. ACS Nano 12, 3975-3984 (2018)

[2] Y. Ma, H.C. Diaz, J. Avila, C. Chen, V. Kalappattil, R. Das, M.-H. Phan, T. Čadež, J.M.P. Carmelo, M. C Asensio, M. Batzill. Angle resolved photoemission spectroscopy reveals spin charge separation in metallic MoSe2 grain boundary. Nat. Commun. 8, 14231 (2017)

[3] P.M. Coelho, H‐P. Komsa, K. Lasek, V. Kalappattil, J. Karthikeyan, M‐H. Phan, A.V. Krasheninnikov, M. Batzill. Room‐Temperature Ferromagnetism in MoTe2 by Post‐Growth Incorporation of Vanadium Impurities. Adv. Electr. Mater. 5, 1900044 (2019).

[4] K. Lasek, M. Ghorbani-Asl, V. Pathirage, A.V. Krasheninnikov, M. Batzill. Controlling Stoichiometry in Ultrathin van der Waals Films: PtTe2, Pt2Te3, Pt3Te4, and Pt2Te2. ACS Nano doi.: 10.1021/acsnano.2c04303 (2022).

標題：IIS-Kavli IPMU-ISSP Joint Seminar：Pseudo-hermitian Random Matrix Theory: Theory & Practice
日時：2022 年 6 月 28 日(火) 午後 1 時 30 分～午後 2 時 30 分
場所：ハイブリッド開催（Zoom および物性研究所本館 6 階 大講義室 A632）
講師：Prof. Joshua Feinberg
所属：University of Haifa
要旨：

Pseudo-hermitian random matrices form a new class of matrix models lying between the classical Wigner-Dyson ensembles of hermitian matrices and the non-hermitian Ginibre ensembles. These matrices are hermitian with respect to an indefinite metric over some vector space. Consequently, their eigenvalues are either real or come in complex conjugate pairs.

Ensembles of pseudo-hermitian random matrices could be thought of probability measures over generators of the non-compact classical Lie algebras, in complete analogy to classical hermitian random matrices being probability measures over the classical compact algebras.

In this talk I will explain the physical motivation for pseudo-hermitian random matrix theory and present explicit numerical and analytical results pertaining to the average eigenvalue spectrum of a concrete pseudo-hermitian random matrix model in the large-N limit.

標題：超強磁場下の有機分子性固体におけるトポロジカル物性と電子相関効果
日時：2022 年 6 月 29 日(水) 午前 11～午後 0 時
場所：Online
講師：野本 哲也 特任研究員
所属：強磁場コラボラトリー
要旨：

有機分子と対イオンから構成される有機伝導体は、非従来型超伝導や Mott 絶縁体、電荷ガラス、量子スピン液体などの多彩な物性が観測される物理学的に興味深い物質である。中でもα型と呼ばれる有機伝導体は Dirac 型の線形分散バン

ドを有するトポロジカル物質の候補として知られ、”質量の無い”電子に由来する特異な電子物性に注目が集まっている[1]。私たちはこのα型有機伝導体の一つ、α-(BEDT-TSF) 2 I 3 をターゲットとした超強磁場中の物理現象について研究を行っている。本物質は強い電子相関により電荷秩序絶縁体へと金属－絶縁体転移を起こす(T MI = 50 K)と考えられてきた物質であるが、近年行われた分光測定や理論的検証により [2]、電子相関に駆動される特殊なトポロジカル絶縁体状態(トポロジカル Mott 絶縁体)が実現している可能性が指摘されている [3, 4]。最近、パルス強磁場を用いた輸送測定により、α-(BEDT-TSF) 2 I 3 のトポロジカル状態に由来すると考えられる巨大磁気抵抗効果などの異常な輸送特性の観測に成功した。本セミナーではこの物質が強磁場中で示す特異な物性を中心に紹介し、有機分子性固体におけるトポロジカル物性の可能性について議論した。

[1] N. Tajima, S. Sugawara, M. Tamura, Y. Nishio, K. Kajita, Journal of the Physical Society of Japan 75(5), 05101 (2006).
[2] S. Kitou et al., Physical Review B 103, 035135 (2021).
[3] S. Raghu, X. L. Qi, C. Honerkamp, S. C. Zhang, Physical Review Letter 100, 156401 (2008).
[4] D. Ohki, K. Yoshimi, A. Kobayashi, Physical Review B 105, 205123 (2022).

標題：Microscopic investigation of chiral crystals
日時：2022 年 7 月 1 日(金)　午後４時～午後５時
場所：On Zoom and Main Lecture Room (A632) at ISSP
講師：Hiroaki KUSUNOSE
所属：Meiji University and ISSP
要旨：

Chirality is a three-dimensional geometric property which is characterized by the absence of any mirror and inversion symmetry operations. Ten of the thirty-two crystallographic point groups belong to this category, and they must have a time-reversal (T) even pseudoscalar representation [1]. A concrete microscopic representation of the chirality is an electric-toroidal (ET) monopole, G0, which becomes active under proper rotations only [2].

Although a monopole seems to be featureless, the pseudoscalar nature cannot be described by a point-like degree of freedom, implying that it has internal degrees of freedom. Indeed, from symmetry point of view, we can decompose G0 as (R1 x R2)・R3 or (M1 x M2)・R3 and so on, where Ri and Mi are independent electric and magnetic dipoles. In these expressions, the vector products are axial vector which suggests that chiral crystal is able to convert between axial and polar quantities through such internal degrees of freedom.

In order to elucidate such a parity conversion property in chiral crystals, we construct the tight-binding model for the typical chiral system of elemental Te and investigated the microscopic expressions of G0 and possible parity conversion responses, namely, electric-field induced rotation and its inverse responses based on the model [3]. We found that the nearestneighbor spin-dependent imaginary hopping is essential ingredient of chirality and is responsible for the electric-field induced lattice rotation and its inverse process.

The conjugate field of G0 (the spin-dependent imaginary hopping) is the combined fields such as the electric current and magnetic field which must be parallel with each other. Along this line, we discuss that the sign of the product of these quantities can control the preferred handedness of chiral crystals, i.e., absolute enantioselection.
We would like to thank J. Kishine, H. Yamamoto, Y. Togawa, Y. Kato, J. Kishine, A. Kato for fruitful discussions.

[1] L.D. Barron, “Molecular Light Scattering and Optical Activity”, 2nd ed. (Cambridge University Press, 2004).
[2] S. Hayami, M. Yatsushiro, Y. Yanagi, and H. Kusunose, Phys. Rev. B, 98, 165110 (2018).
[3] R. Oiwa and H. Kusunose, arXiv:2203.15192.

標題：磁気スキルミオン格子の生成と構造制御
日時：2022 年 7 月 6 日(水) 午後 4 時～午後 5 時
場所：Online
講師：高木 里奈
所属：東京大学大学院 工学系研究科 総合研究機構（物理工学専攻）助教
要旨：

近年、トポロジーの概念を基軸とした物性研究が盛んに行われている。特殊なトポロジーを持つスピン構造である磁気スキルミオンは、粒子としての性質を有し、次世代の磁気メモリにおける情報担体の候補として注目されている。スキルミオンはこれまで空間反転対称性の破れた結晶構造の下で安定化されることが知られてきた。一方、最近では空間反転対称性の保たれた希土類合金中で、従来と比べて一桁小さいナノサイズのスキルミオンが発見され、その起源として遍歴電子に由来する形成機構が新たに提案されている。

私たちは後者の形成機構が働くような新物質探索を進めており、最近、空間反転対称性を有する遍歴磁性体 $EuAl_4$ においてナノサイズのスキルミオン格子状態を発見し、磁場や温度によってスキルミオン格子が正方格子、菱形格子と構造相転移することを見出した。これまでは結晶格子と同じ対称性を持つスキルミオン格子状態のみが観測されていたのに対し、今回の物質ではスキルミオンの配列の自由度があることが明らかとなった。本発表では、ナノサイズのスキルミオン格子の生成とその構造制御について議論するとともに、準安定スキルミオン格子の構造相転移に関する研究も紹介した。

標題：Exotic structures and dynamics of frustrated cholesteric blue phases
日時：2022 年 7 月 8 日(金) 午後 4 時～午後 5 時
場所：物性研究所本館 6 階 大講義室（A632）とオンライン（Zoom）のハイブリッド形式
講師：福田 順一
所属：九州大学
要旨：

Cholesteric blue phases (BPs) are complex three-dimensional structures exhibited by a chiral liquid crystal. BPs comprise a regular array of line defects of orientational order (disclination lines) and double-twist cylinders where the orientational order is twisted along all the directions perpendicular to the cylinder axis. BPs have attracted the interest of physicists as a fascinating example of order induced by frustration, here between the locally favorable double-twist ordering, and global constraints that prohibits double-twist ordering to fill the whole space without singularities.

In this talk we present two studies on how geometric frustrations affect the structures of already frustrated BPs. One concerns the behavior of BPs confined by two parallel flat substrates. The interaction between confining surfaces and the liquid crystal (surface anchoring) frustrates the ordering of BPs, and numerical calculations based on a continuum theory demonstrate the formation of various exotic structures not found in bulk BPs. We particularly focus on the formation of half-Skyrmions, swirl-like order without singularity that has been found in diverse condensed matter systems. We discuss the dynamics of half-Skyrmions driven by thermal fluctuations, and how they are observed experimentally.

The other subject is on the frustration by the mismatch of the lattice orientations of BP leading to twin boundaries. Twinning of BPs like martensites has been revealed in recent experiments, but real-space fine structures of twin boundaries are difficult to observe experimentally. Again systematic numerical calculations based on a continuum theory clarify how two BP lattices with different lattice orientation should be connected. We also present our recent attempts towards the dynamics of phase transition associated with twin formation.

References:
A. Nych, J. Fukuda et al., Nature Phys. 13, 1215 (2017).
J. Fukuda et al., Ann. Phys. 534, 2100336 (2022) (Review article).
A. Yamashita and J. Fukuda, Phys. Rev. E 105, 044707(1-9) (2022).

標題：空間反転対称性の破れた磁性体における非相反輸送現象とその逆効果
日時：2022 年 7 月 15 日(金)　午前 11 時～午後 0 時
場所：Online
講師：新居 陽一
所属：東北大学金属材料研究所
要旨：

空間反転対称性と時間反転対称性が同時に破れた物質では、電子や光の性質が進行方向によって異なる非相反現象が生じることがある。主に光や電子を舞台として研究されてきたが、最近ではシフト電流やマグノン・フォノン・超伝導の非相反性など様々な観点で研究されてきている。本セミナーでは、最近の我々の成果として熱流やフォノンにおける非相反輸送現象や非相反性の逆効果を用いて磁化やキラリティを制御した成果などに関して発表した。

標題：因果主導機能分解ネットワーク生成手法のデータスキーマ作成への適用
日時：2022 年 7 月 15 日(金)　午後 4 時～午後 5 時
場所：物性研究所大講義室（A632）及び Zoom（ハイブリッド開催）
講師：木野 日織
所属：（国）物質・材料研究機構
要旨：

実験、理論計算で生成されたデータを再利用するためにデータを FAIR 原理に従い公開するオープンサイエンスの推進は世界的な流れである。データを公開するには共通した・もしくは相互変換可能なデータスキーマ（何をどの型で入れるのか）を用いて公開することが望ましいが、それ以前にデータスキーマ自体に対しては、新規手法に対してもスキーマの追加が容易に行えるような手法の基に作成することが望ましい。

多くのデータスキーマは参照を容易にするように階層構造を成す。このデータスキーマ作成の手法の一つに暗黙知を顕在化し概念を分解するオントロジーがある。オントロジーとは逆に、具体的な目的達成のために暗黙知である機能と手法を顕在化し、知識を統合する因果主導機能分解ネットワーク及び関連手法である対象物属性フローチャート[1]を用いてもデータスキーマとして利用可能な語彙の階層・ネットワーク構造を作成可能である。本セミナーでは第一原理プログラム AkaiKKR そして入出力解析スクリプト PyAkaiKKR に対して適用しデータスキーマを作成した例を紹介した[2]。

標題：The theory of the non collinear kagome antiferromangets and its implications
日時：2022 年 7 月 20 日(水)　午後 3 時～午後 4 時
場所：Zoom および大講義室（A632), ISSP（ハイブリッド開催）
講師：Dr. Sayak DASGUPTA
所属：The University of British Columbia and ISSP
要旨：

We construct a field-theoretic description of spin waves in hexagonal antiferromagnets with three magnetic sublattices and coplanar 1200 magnetic order [1]. The three Goldstone modes can be separated by point-group

symmetry into a singlet α0 and a doublet β. The α0 singlet is described by the standard theory of a free relativistic scalar field. The field theory of the β doublet is analogous to the theory of elasticity of a two-dimensional isotropic solid with distinct longitudinal and transverse “speeds of sound.” The speeds of sound can be readily calculated for any lattice model. We apply this approach to the compounds of the Mn3X family with stacked kagome layers and extract the exchange coefficients for a model spin Hamiltonian by fitting to neutron scattering data [2]. We then extend our studies to the case of strained system where we show that strain can be used to tune the magnetism and the Hall response of these compounds in both static and dynamic conditions [3,4].

Refs:
[1] S. Dasgupta and O. Tchernyshyov, Phys. Rev. B 102, 144417 (2020)
[2] Y. Chen et al Phys. Rev. B 102, 054403 (2020)
[3] M. Ikhlas, S. Dasgupta et al, Nature Physics (2022) (accepted)
[4] S. Dasgupta, O. Tretiakov, Communications Physics (in review)

標題：光フィードバックによる共鳴トンネルダイオード発振器のモード同期発振
日時：2022 年 7 月 20 日(水)　午前 10 時 30 分～午後 0 時
場所：第 1 会議室＋Zoom
講師：平岡 友基
所属：Bielefeld University
要旨：

共鳴トンネルダイオード(RTD)発振器は、半導体量子井戸である RTD をゲインとして利用した発振器である。電子発振器として最高周波数の 1.98 THz までの連続波発振[1]が可能であり、低コスト・高効率・室温動作可能であることから、将来のテラヘルツ通信などにおけるテラヘルツ光源として有望なデバイスである。

我々は、テラヘルツ光の注入[2]、出力光を発振器自身に戻す光フィードバック[3]といった外部擾乱に対する非線形応答に注目して RTD 発振器の特徴を明らかにしてきた。本講演では主に、光フィードバックによって RTD 発振器がモード同期発振を示し、テラヘルツ周波数コムを発生することを明らかにした研究について紹介する [3]。本研究では、モード同期状態におけるテラヘルツ波形が周波数変調的であることを実験的に明らかにし、また RTD 内部での電子の走行時間に対応する RTD の非線形容量がモード同期を引き起こしていることを回路シミュレーションで示した。

[1] Izumi, R., Suzuki, S. & Asada, M. 1.98 THz resonant-tunneling-diode oscillator with reduced conduction loss by thick antenna electrode. in 2017 42nd International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz) 1–2 (ieeexplore.ieee.org, 2017).
[2] Hiraoka, T. et al. Injection locking and noise reduction of resonant tunneling diode terahertz oscillator. APL Photonics 6, 021301 (2021)
[3] Hiraoka, T., Inose, Y., Arikawa, T. Ito, H., and Tanaka, K. Passive mode-locking and terahertz frequency comb generation in resonant-tunneling-diode oscillator, Nat. Commun., in press (Preprint: https://doi.org/10.21203/rs.3.rs-919266/v1).

標題：Classical vs Quantum Heisenberg kagome antiferromagnet materials: an experimental perspective from spectroscopic techniques

日時：2022 年 7 月 21 日(木) 午後４時～午後５時

場所：第５セミナー室（A615）及び Zoom（ハイブリッド開催）

講師：Edwin Kermarrec

所属：Université Paris-Saclay

要旨：

The Heisenberg Kagome Antiferromagnet (HKAF) model occupies a central place in the field of magnetic frustration. Very early on, pioneering theoretical studies highlighted its specificity even at a classical level [1]. The quantum case is even more intriguing, with a quantum spin liquid ground-state characterized by long-range entanglement and fractionalized excitations.

In this talk, I will briefly introduce the physics inherent to the Heisenberg kagome antiferromagnet and report our recent work on two new kagome materials, using complementary spectroscopic probes (NMR, muSR and inelastic neutron scattering) to investigate their spin excitations.

The first one is a classical KHAF, the S=5/2 layered monodiphosphate Li9Fe3(P2O7)3(PO4)2 [2]. Thanks to the moderate exchange interaction (J ~ 1 K) between spins, we could experimentally investigate the phase diagram of the classical model under applied fields and evidence the highly sought-after 1/3rd magnetization plateau in a kagome compound. The second one is the S=1/2 quantum KHAF Y3Cu9(OH)18OCl8, the most recent derivative of the emblematic Herbertsmithite, which does not show any dilution or interlayer defects. The slight distortion of its kagome lattice creates three symmetry-inequivalent antiferromagnetic couplings. This S=1/2 anisotropic KHAF model was recently found to host a rich phase diagram with spin-liquid and ordered ground states [3]. I will present the results of our recent investigation using NMR, μSR and neutron scattering techniques performed on single crystals [4].

[1] J. T. Chalker, P. C. W. Holdsworth, & E. F. Shender, Phys. Rev. Lett. 68, 855 (1992).

[2] E. Kermarrec, R. Kumar, G. Bernard, R. Hénaff et al., Phys. Rev. Lett. 127, 157202 (2021).

[3] M. Hering et al., npj Comput. Mater 8, 10 (2022).

[4] D. Chatterjee et al., unpublished

標題：Imaginary-time evolution algorithm on quantum computers and its perspective on quantum chemical calculations

日時：2022 年 7 月 25 日(月) 午後４時～午後５時

場所：Online

講師：松下 雄一郎

所属：東京工業大学 物質・情報卓越教育院

要旨：

Currently, quantum chemical calculations using quantum computers are attracting a great deal of attention. We have been developing algorithms for quantum chemical calculations using quantum computers. In particular, we have recently focused on the imaginary-time evolution method. Note that algorithms using quantum computers must be expressed in terms of unitary operations and observations for each qubit. Therefore, it was a nontrivial problem how to perform the imaginary-time evolution operator, which is a non-unitary operation, on a quantum computer. We have developed a method to implement the imaginary-time evolution algorithm in a form using auxiliary bits and proposed a method of first-quantized eigensolver for quantum chemistry for ground states based on the imaginary-time

evolution method [1]. Furthermore, we have been working on developing algorithms to reduce errors when performing calculations on quantum computers [2]. In this presentation, we will discuss the fundamentals of quantum computers, the implementation of the imaginary-time evolution algorithm, the computational cost of implementing the imaginary-time evolution algorithm for materials calculations, and the error mitigation algorithms we have been developing.

[1] T. Kosugi, Y. Nishiya, and Y. Matsushita, arXiv: 2111.12471 (2021). To be published in Physical Review Research.
[2] Y. Hama and H. Nishi, arXiv: 2205.13907 (2022).

標題：Variational Tensor Network Operator
日時：2022 年 8 月 1 日(月)　午後 1 時～午後 2 時
場所：Online
講師：Yu-Hsueh Chen
所属：National Taiwan University
要旨：

We propose a simple and generic construction of the variational tensor network operators to study the quantum spin systems by the synergy of ideas from the imaginary-time evolution and variational optimization of trial wave functions. By applying these operators to simple initial states, accurate variational ground state wave functions with extremely few parameters can be obtained. Furthermore, the framework can be applied to study spontaneously symmetry breaking, symmetry protected topological, and intrinsic topologically ordered phases, and we show that symmetries of the local tensors associated with these phases can emerge directly after the optimization without any gauge fixing. This provides a universal way to identify quantum phase transitions without prior knowledge of the system.

標題：Photoexcited nonequilibrium dynamics in an excitonic insulator candidate Ta2NiSe5 explored by pump-probe Raman and luminescence spectroscopy
日時：2022 年 8 月 4 日(木)　午前 10 時 30 分～午後 0 時
場所：Room #D120 in ISSP + Zoom (hybrid)
講師：Kota Katsumi
所属：Université Paris Cité
要旨：

In narrow gap semiconductors or semimetals, the Coulomb interaction between electrons and holes may lead to a spontaneous formation of excitons. These excitons are expected to condense and give rise to an unconventional insulating ground state called excitonic insulator [1]. Among the various exitonic insulator candidate materials, Ta2NiSe5 is a prototypical example because it has a direct band gap and has no instability at finite wave-vector, such as charge density wave order [2]. As the temperature is lowered, Ta2NiSe5 displays a semiconductor-to-insulator (SI) transition below the transition temperature Tc = 325 K, which is associated with an excitonic insulator transition due to electronic correlations [2,3,4]. However, the origin of the SI transition has been still elusive because it is accompanied by a structural transition from orthorhombic to monoclinic symmetry [5]. To study whether the SI transition is lattice or electronic-driven, pump-probe optical spectroscopy is a promising technique because it can track the electronic and lattice responses separately.

In this study, we first performed equilibrium emission spectroscopy for Ta2NiSe5. In addition to low-energy electronic and phononic Raman excitations, we found significant photoluminescence (PL) signal whose intensity

sharply increases below Tc, which we assign to enhanced electron-hole interactions in the insulating phase. We further investigated the pump-probe Raman and PL intensity after photoexcitation, where the Raman and PL signals serve as reporters of the lattice symmetry and the insulating gap, respectively. In this talk, we will discuss the results of the pump-probe measurements in light of the lattice-driven versus electronic-driven scenario for the SI.

[1] D. J´erome et al., Phys. Rev. 158, 462 (1967)
[2] Y. Wakisaka et al., Phys. Rev. Lett. 103, 026402 (2009)
[3] K. Seki et al., Phys. Rev. B 90, 155116 (2014)
[4] Y. F. Lu et al., Nat. Commun. 8, 14408 (2017)
[5] F. J. Di Salvo et al., Journal of the Less Common Metals 116, 51 (1986)

標題：有限温度におけるフォノンと結晶構造の第一原理計算：自己無撞着フォノンによるアプローチ
日時：2022 年 8 月 19 日(金) 午後 4 時～午後 5 時
場所：物性研究所本館 6 階 大講義室（A632）とオンライン（Zoom）のハイブリッド形式
講師：只野 央将
所属：国立研究開発法人物質・材料研究機構
要旨：

First-principles structural optimization and phonon calculation based on density functional theory (DFT) are widely used and indispensable in modern materials science study. While these approaches are quite powerful for predicting ground state properties, predicting finite-temperature structures and phonons remains challenging because various elementary excitations, particularly phonons, and their temperature dependence need to be considered. In this seminar, we present a self-consistent phonon (SCP) theory [1] and its extension as an effective way to access finite-temperature phonons and structures. We discuss the accuracy and efficiency of the SCP approaches by showing our recent results on CsPbBr3 [2] and BaTiO3 [3].

[1] T. Tadano and S. Tsuneyuki, Phys. Rev. B 92, 054301 (2015).
[2] T. Tadano and W. A. Saidi, arXiv:2103.00745.
[3] R. Masuki, T. Nomoto, R. Arita, and T. Tadano, arXiv:2205.08789.

標題：Classification of classical spin liquid in the large-S limit
日時：2022 年 8 月 22 日(月) 午後 1 時 30 分～午後 2 時 30 分
場所：柏図書館メディアホールおよび Zoom
講師：Dr. Han Yan
所属：Rice University
要旨：

Classical spin liquids are arguably one of the most interesting types of classical matter. They are described often by the classical limit of gauge theories (electrostatics) and can be upgraded to topological orders or gapless quantum liquid states if equipped with proper quantum dynamics. In this work, we present a classification scheme for classical spin liquids in the large-S limit. In this limit, the spin components are effectively real scalars, so the spectrum of the Hamiltonian accurately describes its properties. We found that the ground state degeneracy corresponds to flat bands at the bottom of the spectrum, and the flat band's structure crucially decides the physics of the classical spin liquid. When there is a singular band-touching between the top bands and the bottom flat ones, the system has algebraic

correlation. The ground state is then described by a generalized Gauss's law, whose algebraic form is determined by the band touching structure. A much less studied category is when the flat bands are gapped from the top ones. In this case, the correlation is short-ranged, but the classical spin liquid can be distinguished from a trivial paramagnet by the fragile topological homotopy of the bottom bands. Besides building the general mathematical framework of the classification, I will also show some concrete examples and discuss experimental applications.