

物性研究

標題: AI meets Theoretical Physics: machine learning assisted solution of a difficult problem in frustrated magnetism

日時：2024年6月10日(月) 午後4時～午後5時

場所：物性研究所本館 6 階 第 5 セミナ一室 (A615)

講師：Prof. Nic Shannon

所属：Okinawa Institute of Science and Technology

要旨：

Much has been made of the potential of AI to revolutionize the workplace. The range of tasks which can be performed by machines is expanding rapidly, and in many easily-defined tasks, such as playing chess, machines now comfortably out-perform humans. AI also brings the opportunity to automate many of the routine, repeated, tasks which arise in scientific research. But how AI will impact on the creative, conceptual, and problem-solving aspects of science, remains an open question.

In this talk we examine how AI contributed to the solution of a difficult problem in frustrated magnetism: the phase transition from a spin liquid described by a tensor gauge theory into a previously unknown form of magnetic order. This problem, which had defied conventional numerical simulation, was solved through a generative use of support vector machine (SVM), without prior training on related problems. However, neither the contributions of the SVM, nor that of the human researchers, proved decisive by themselves. Rather, success followed from a process resembling a collaboration between man and machine. We argue that this kind of “collaboration” may become the norm, especially in research involving large sets of data.

- [1] “Identification of emergent constraints and hidden order in frustrated magnets using tensorial kernel methods of machine learning” J. Greitemann et al., Phys. Rev. B 100, 174408 (2019).
- [2] “Human-machine collaboration: ordering mechanism of rank-2 spin liquid on breathing pyrochlore lattice”, N. Sadoune et al., arXiv:2402.10658

標題：Theory, prediction and detection for topological and chiral phonons

日時：2024年6月10日(月) 午前10時～

場所：物性研究所本館 6 階 第 5 セミナ一室 (A615)

講師：Prof. Tiantian Zhang

所属: Theoretical Institute of Physics, Chinese academy of sciences, Beijing, China

要旨：

The effective control of phonon cannot only provide a new perspective for the understanding of physical processes such as thermal conductivity and electroacoustic coupling, but also promote the realization of related applications. However, the fundamental properties of “zero spin” and electrical neutrality make the means of manipulation of phonons very limited. Around 2018, with the popularization of topological band theory to solid phonon spectrum, and the establishment of a first-principles method to calculate topological phonon in real material systems [1], the degree of freedom of “topology” was successfully introduced into phonon systems, and it offers a way to modulate phonons. In the first part of the talk, I will introduce the theoretical and experimental results of several topological phonon

materials, such as the double-Weyl phonon material FeSi [1-2], the twofold quadruple Weyl phonon material BaPtGe [3-4], and the node-line phonon material MoB2 [5].

In addition to “topology”, phonon can also have a degree of freedom called “chirality”. For example, chiral phonons with non-zero circular polarization play an important role in the inter/intra-valley scattering of electron valleys and the light selection transition in the system that breaks the time-space inversion symmetry. However, in the past, most of the studies on chiral phonons were limited to two-dimensional systems, and the carrying group velocity was zero, which is not conducive to the practical application of chiral phonon in information dissemination [6]. Therefore, the second part of the report focuses on extending chiral phonon research to three-dimensional chiral crystal systems [7], and verifies the existence of chiral phonon at the center of BZ with high group velocity in α -HgS and elemental Te [8-9]. Finally, the talk will also explore the relationship between Weyl phonon and chiral phonon [9], as shown in the Figure below.

標題：高分解能レーザー励起光電子顕微鏡を使った物性研究

日時：2024年6月13日(木) 午後4時～午後5時

場所：物性研究所本館 6 階 第 5 セミナ一室 (A615)

講師：谷内 敏之

所属：東京大学 マテリアルイノベーション研究センター・新領域創成科学研究科

要旨：

光電子顕微鏡(PEEM)は一般的な電子顕微鏡とは異なり、励起源として光を利用することにより、物性の情報を直接可視化できる顕微手法であり、非破壊・電子状態に敏感なコントラスト・適度な検出深さ・高いスループットといった特長を持っている。特に光源の波長と偏光性を制御することで物質中の元素・価数・原子/分子配向・キャリア濃度・電子スピンといった様々な電子状態の可視化が可能な強力なツールとして基礎研究での顕微手法として利用されている。しかしながら PEEM は空間分解能が最高で 10 nm 程度、通常は 20 nm と他の電子顕微鏡と比較しかなり劣っていた。講演者は、PEEM の分解能を制限している主な要素は電子レンズ系の球面収差・色収差、および放出した光電子の空間電荷効果であることを明らかにし、電子ミラー型の収差補正器と連続波の深紫外レーザーを組み合わせたシステム(レーザー PEEM)を建設した。またレーザー光源には光強度 1017 photons/s、光子エネルギー4.66 eV のレーザーを用いることで世界最高となる空間分解能 2.6 nm を達成した[1]。

本講演では装置開発に加え、レーザーPEEMを用いた応用研究例を紹介する。上述のレーザー光源では放出される光電子の運動エネルギーが非常に小さいため(閾値光電子)、光電子が物質中を伝搬する距離(平均自由行程)が大きくなる。これにより厚さ 10 nm 以上の材料の下に埋もれたナノ構造を高い分解能で可視化することも可能である。埋もれたナノ構造観察の実施例として、上部にキャップ層が堆積された磁性薄膜、および酸化物ヘテロ界面で特異に発現する界面強磁性相の磁気イメージング、また電子デバイス構造の非破壊観察を試みたのでその結果を紹介しつつ、レーザーPEEMの可能性について議論した。

Lab tour (semi-autonomous PLD tools)

If a physical system is perturbed from equilibrium, the rate that it equilibrates is an important measure of its physics. In condensed matter physics, we are used to measuring such rates in the context of linear response to electromagnetic fields. For instance, the rate that current decays in a metal after an electric field impulse can be related to the width of its low-frequency “Drude” response in the optical conductivity. The rate that polarization decays after polling a liquid with an E field corresponds to the width of the broad peak in the Debye relaxational functional form. In contrast, the rate of energy relaxation is a fundamental rate that governs many processes in solids, but which is unfortunately not measured straightforwardly via conventional electrodynamic linear response. However quite generically, this rate can be measured in various non-linear χ_3 spectroscopies. I will discuss recent technical developments in the form of THz range 2D coherent spectroscopy (and its relatives) that allow us to get new information about energy relaxation in correlated and topological metals, as well as disordered electron glasses. I will discuss a number of systems and phenomena in which unconventional dynamics and energy relaxation govern their low energy behavior. I will give number of examples of the power of these new techniques to strongly interacting metals, Dirac semimetals, collective modes in superconductors, electron glasses, and 1D spin chains.

T.Ozaki has recently developed a new method to construct the closest Wannier (CW) orbitals to a given set of localized guiding orbitals [1]. In the CW formalism, the disentanglement of bands is achieved with no iterative calculations, significantly reducing computational costs. In this talk, I will present a generation scheme of the CW

標題：Machine Learning for Quantum Materials

日時：2024 年 6 月 24 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) および Online

講師：Prof. Eun-Ah Kim

所属：Cornell University

要旨：

Decades of efforts by the quantum materials research community drove a “data revolution.” Modern experimental modalities produce high-dimensional data in large volumes. Unprecedented control and new facilities imply new dimension and new knobs, such as time-resolved probing or scanning probing. Moreover, massive amounts of high-throughput ab-initio data and curated experimental data are becoming accessible to researchers. Much needed are data-centric approaches that accelerate discoveries from these data through synergetic interaction with expert human researchers’ insights. A synergy between data science and quantum materials research is essential for such endeavors to result in scientific progress. I will present cases of fruitful collaborations that led to new insights and started to shape an approach to data sets of the new era. Specifically, I will discuss how to use unsupervised learning to discover new physics from large volumes of evolving data and how to use supervised learning to uncover descriptors of emergent properties from limited volume of expertly curated data. If time permits, I will discuss new efforts to using language models for routine calculations such as Hartree-Fock mean field theory.

標題：Non-Abelian Hopf-Euler insulators

日時：2024 年 6 月 26 日(水) 午前 10 時～

場所：物性研究所本館 6 階 第 5 セミナー室 (A615)

講師：Morris, Arthur Samuel

所属：King’s College, University of Cambridge, Cambridge

要旨：

Many free-fermion topological phases of matter such as the Chern insulator are characterised by topological quantum numbers assigned to single isolated bands. While such single-band phases are now well understood, intriguing features remain to be explored within topological band theory. I will explain how nodes in real Bloch Hamiltonians carry non-Abelian topological charges which arise from the geometry of the classifying space. Moreover, by braiding these nodes around each other in reciprocal space, it is possible to induce a ‘multi-band’ topological phase, where the two band subspace supporting the nodes is labelled with an integer, the Euler class. Another example of a multi-band topological invariant is the Hopf invariant, which characterises three dimensional complex phases and provides a solid state realisation of the Hopf fibration. Such systems can also host Chern numbers on each coordinate plane within the Brillouin zone; I will describe how the presence of such subdimensional invariants influences the bulk Hopf invariant. Finally, I will discuss a real topological phase in 3D which possesses a bulk Hopf invariant and 2D Euler classes. These systems have nontrivial quantum geometry, and appear to host unusual nodal line structures.

[1] arXiv:2405.17305 (2024).

[2] Nat. Phys. 16, 1137–1143 (2020).

[3] Phys. Rev. Lett. 101, 186805 (2008).

[4] Phys. Rev. B 94, 035137 (2016).

[5] Phys. Rev. B 108, 125101 (2023).

標題：Network topology reveals robust adaptation phenomena in biochemical systems

日時：2024年6月28日(金) 午後4時～午後5時

場所：物性研究所 6 階第 5 セミナー室 (A615) 及び Online (Hybrid)

講師：広野 雄士

所属：大阪大学

要旨：

Maintaining stability is a critical issue for living systems. Robust perfect adaptation (RPA) is a control-theoretical mechanism that enables certain output variables to attain and sustain desired values despite external disturbances in a robust manner. RPA helps the survival of living systems in unpredictable environments, and as such there are numerous examples of biological implementations of this feature. However, identifying RPA properties and associated regulatory mechanisms is a highly nontrivial problem given the complexity of biological systems.

In this talk, we aim to elucidate the essential role of network topology in the phenomenon of RPA [1]. We have recently shown that the RPA properties in a deterministic chemical reaction system can be characterized by topological characteristics of subnetworks. This connection allows us to enumerate all the RPA properties implemented in a reaction network efficiently. Furthermore, we explicitly identify the integral controllers that work in concert to realize each RPA property.

Reference:

[1] Yuji Hirono, Ankit Gupta, Mustafa Khammash,

“Complete characterization of robust perfect adaptation in biochemical reaction networks.”

標題：Witnessing Disorder in Spin Chains

日時：2024年7月3日(水) 午前10時～午前11時

場所：物性研究所本館 6 階 第 5 セミナ一室 (A615)

講師 : Snigdha Sabharwal

所属 : Okinawa Institute of Science and Technology

要旨：

There are no clean samples in nature. Therefore, can one meaningfully quantify the effects of disorder on the entanglement structure of quantum states? In this talk, we investigate the entanglement structure of Tomonaga-Luttinger liquids (TLL) and random singlet (RS) states in an antiferromagnetically interacting Heisenberg spin chain. We make use of entanglement witness based measures like concurrence, tangle and quantum Fisher information (QFI), for this task, which can be related to experimentally accessible observables like spin correlations. Using quantum Fisher information (QFI), we demonstrate that both TLL and RS states exhibit multipartite entanglement. This result for the RS state, we attribute to the localization of multipartite entanglement below the crossover length. Additionally, we show that the order of disorder average matters for measures like concurrence and tangle, and this can lead to false inferences when ruling out RS states. Finally, we show that the low-temperature behavior of these witnesses can be utilized to characterize the effects of disorder. From the low-temperature behavior of concurrence, we extract the central charge information for the TLL state and conjecture this could be done for the RS state as well. Furthermore, using the equal-time structure factor as a multipartite entanglement witness, we demonstrate a distinct growth in multipartite entanglement in the two states.

標題：Exploring Membrane Topology Transformations using Polymer Field Theory

日時：2024年7月5日(金) 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 号室)及び Online (Hybrid)

講師：Dr. Russell Spencer

所属：ゲッティンゲン大学

要旨：

Membrane remodeling, including fusion and fission, plays a crucial role in various cellular processes. However, understanding the intricacies of these topological changes can be challenging due to the involvement of large-scale membrane rearrangements and their sensitivity to small-scale molecular behavior. Moreover, these remodeling events face significant free-energy barriers that necessitate the presence of catalytic proteins. In this work, we utilize self-consistent field theory (SCFT) in combination with the string method to identify the Minimum Free Energy Path (MFEP). We thereby determine the most probable pathway for specific remodeling transitions implicated in cellular signaling and organelle division. This approach has allowed us to discover a new pathway by which the fusion of membranes may catalyze their fission. Furthermore, we extend conventional SCFT methods, introducing proteins inspired by the dynamin family. These proteins facilitate fission by constricting membrane tubes. We find that the free energy barrier to fission depends strongly on membrane tension and constriction. In addition to simply constricting the membrane, dynamin’s PH domains are inserted between lipid head groups, inducing membrane distortion. Our results emphasize the crucial role of this distortion in reducing the free energy barrier to fission. This research sheds light on the underlying mechanisms of membrane remodeling and provide insights into cellular processes involving topological changes.

標題：SO(5)-symmetric deconfined quantum critical point in the extended JQ-model

日時：2024年7月12日(金) 午後4時～午後5時

場所：物性研究所本館 6 階 第 5 セミナ一室 (A615)

講師：高橋 惇

所属：東京大学物性研究所

要旨：

Since its original proposal [1], the existence and microscopic realization of deconfined quantum critical (DQC) points with lattice models has been under extensive debate. Field-theoretic arguments for DQC provide a plausible scenario where the quantum phase transition between a Neel phase and a valence-bond solid phase — two most basic phases of matter in quantum magnetism — will generically be critical (and is dubbed DQC), despite the fact that they are both spontaneous symmetry breaking phases with a priori completely unrelated symmetries. The so-called JQ model has always been a prominent candidate for a microscopic model exhibiting DQC, but anomalous finite-size scalings and violations with conformal bootstrap bounds had hindered conclusive resolution.

In this talk, I will present our recent efforts to clarify this situation. By examining various correlation functions in the JQ model, we show that the DQC point actually has an additional relevant field, which implies the need for extra parameter tuning to arrive at the true DQC point [2]. After observing a clearly first-order transition with emergent SO(5) symmetry in a related JQ-type model [3], we recently conducted a large-scale numerical experiment for the JQ model with an additional parameter that extends the phase diagram [4]. Our results are consistent with the existence of an SO(5) symmetric DQC point in the extended JQ model phase diagram, but only in the sign-problematic region for quantum Monte Carlo. Although the true DQC point is not directly observable, we show how the extrapolated critical exponents match very well with recently calculated values from sophisticated conformal field theoretic fuzzy

sphere calculations [5].

- [1] T. Senthil et al., Science 303, 1490 (2004).
- [2] B. Zhao, JT, and A. Sandvik, PRL 125, 257204 (2020).
- [3] JT and A. Sandvik, PRR 2, 033459 (2020).
- [4] JT, S. Hui, B. Zhao, W. Guo, and A. Sandvik, arXiv:2405.06607 (2024).
- [5] Z. Zhou, L. Hu, W. Zhu, Y-C. He, arXiv:2306.16435 (2023).

標題：Anomalous crystal shapes of topological materials

日時：2024 年 7 月 16 日(火) 午後 2 時 45 分～午後 3 時 45 分

場所：物性研究所本館 6 階 第 5 セミナー室 (A615)、および Online (ハイブリッド)

講師：田中 悠太郎

所属：国立研究開発法人理化学研究所 創発物性科学研究センター

要旨：

Understanding crystal shapes is a fundamental subject in surface science. It is now well-studied how chemical bondings determine crystal shapes via the dependence of surface energies on surface orientations. Meanwhile, discoveries of topological materials have led us to a new paradigm in surface science, and one can expect that topological surface states may affect surface energies and crystal facets in an unconventional way.

In this talk, we show that the surface energy of glide-symmetric topological crystalline insulators (TCI) depends on the surface orientation in a singular way via the parity of the Miller index. This singular surface energy of the TCI affects equilibrium crystal shapes, resulting in the emergence of unique crystal facets of the TCI [1]. Furthermore, we study the equilibrium crystal shapes of a topological insulator (TI), a TCI protected by mirror symmetry, and a second-order topological insulator (SOTI) protected by inversion symmetry. In terms of the calculations of the simple tight-binding model, we show that the various boundary states of the TI, TCI, and SOTI affect the emergence of the specific facets [2].

Reference

- [1] Y. Tanaka, T. Zhang, M. Uwaha, and S. Murakami, Phys. Rev. Lett. 129, 046802 (2022).
- [2] Y. Tanaka and S. Murakami, Phys. Rev. B 107, 245148 (2023).

標題：General criterion for non-Hermitian skin effects and Fock space skin effects

日時：2024 年 7 月 16 日(火) 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)、および Online (ハイブリッド)

講師：下村 顕士

所属：京都大学 基礎物理学研究所

要旨：

Non-hermiticity of evolution operators appears in a wide range of physics, from classical to quantum systems [1]. Non-Hermiticity enables macroscopic accumulation of bulk states, named non-Hermitian skin effects [2]. They are well-established for single-particle systems, but their proper characterization for general systems is elusive.

In this talk, we propose a general criterion of non-Hermitian skin effects, which works for any finite-dimensional system evolved by a linear operator [3]. The applicable systems include many-body systems. A system meeting the criterion exhibits enhanced non-normality of the evolution operator [4], accompanied by exceptional characteristics

- [1] Y. Ashida, Z. Gong, and M. Ueda, *Adv. Phys.* 69, 249, (2020).
- [2] S. Yao and Z. Wang, *Phys. Rev. Lett.* 121, 086803 (2018).
- [3] K. Shimomura and M. Sato, *arXiv:2403.13595* (2024).
- [4] Y. O. Nakai, N. Okuma, D. Nakamura, K. Shimomura, and M. Sato, *Phys. Rev. B* 109, 144203 (2024).

本講演では、オープンソースライセンスの基盤となる著作権の基本概念を説明し、ソフトウェア開発における主要なライセンスの種類やその特徴、特に物性科学研究においてよく利用されるオープンソースライセンスについて解説した。

To explore such quantum critical picture, we have performed an-plane transport – longitudinal and Hall – measurements on LSCO cuprate near critical doping in a broad range of magnetic fields, up to 90 T. The observed temperature and magnetic field dependence of resistivity reveal scale-invariant behavior where temperature and magnetic field compete to set the infrared cutoff of critical fluctuations. Hall resistivity crosses over to a scale-invariant behavior at very high magnetic fields.

標題：超高速エレクトロニクスを用いたグラフェン電荷ダイナミクスのテラヘルツオンチップ計測

日時：2024 年 7 月 18 日(木) 午前 10 時～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：吉岡 克将

所属：NTT 物性科学基礎研究所

要旨：

超高速レーザー分光技術の発達は、フェムト秒の時間スケールにおいて固体中の電子状態を観測・制御することを可能にした。我々は、そのような超高速応答を使ったデバイスあるいは信号処理の実現に向けて研究を進めている。具体的には、オンチップテラヘルツ分光[1]や酸化亜鉛ゲート構造[2]を応用することで、220 GHz の動作速度に達するグラフェン光検出器による超高速光電変換[3]、さらにはグラフェンにおけるピコ秒電子波束のオンチップ計測によるプラズモン伝搬[4]に成功した。当日は詳細な物理機構についても議論した。

標題：Exploring the interface between biophysics and nonequilibrium statistical physics

日時：2024 年 7 月 19 日(金) 午後 4 時～午後 5 時

場所：物性研究所 6 階第 5 セミナー室 (A615) 及び Online

講師：畠山 哲央

所属：東京工業大学地球生命研究所

要旨：

What biophysics studies are life phenomena, and therefore in most cases they are nonequilibrium. The central topic of statistical physics is also shifting towards nonequilibrium phenomena. However, the connections between biophysics and nonequilibrium statistical physics are still limited. One reason for this is that both fields have increasingly specialized in different directions: In biophysics, experimental techniques allow us to measure increasing amounts of data, so we are able to study more and more complex phenomena, while in nonequilibrium statistical physics, recent developments in mathematical techniques have led to increasingly rigorous mathematical approaches. Thus, few attempts have been made to find “right size” phenomena that can serve as an interface between the two fields. If a theory at the interface is found, the exchange between the two fields will progress and physics may be able to enter a new phase.

In this seminar, I would like to introduce two examples of our attempts to explore the interface between biophysics and nonequilibrium statistical physics. One is the mitochondrial alignment. Mitochondria are critical organelles in eukaryotes that produce the energy currency ATP. In nerve axons, mitochondria are known to align at almost regular intervals to maintain a constant ATP concentration, but little is known about the mechanism. We show that ATP production and ATP-dependent nondirectional movement of mitochondria are sufficient for alignment, even without an explicit repulsive force between them. This is similar to thermodynamic forces driven by thermal fluctuations, even generated by nonequilibrium processes.

Also, I introduce the new theoretical concept, the Enzymatic Mpemba effect. Increasing the enzyme concentration generally speeds up enzymatic reactions. However, I show that increasing the enzyme concentration can also slow down the relaxation to the equilibrium state, and mechanism for this slowing is similar the Mpemba effect.

◇13:00-13:30 佐藤 健 東京大学

Simulations of intense laser-driven multielectron dynamics using classical and quantum computers

◇13:30-14:00 小杉 太一 株式会社 Quemix/東京大学

Efficient qubit encoding using a Lorentzian basis set for molecular orbitals in real space

◇14:00-14:30 明石 遼介 量子科学技術研究開発機構

Eliashberg theory in the uniform electron gas revisited

◇14:30-15:00 鈴木 康光 聖光学院中学校高等学校

Machine learning exchange-correlation potential in time-dependent density-functional theory

◇16:00-17:00 金井 陽介 ノースカロライナ大学

【Theory Seminar】 Coupled Quantum Dynamics of Electrons and Protons in Heterogeneous Environments

標題：Coupled Quantum Dynamics of Electrons and Protons in Heterogeneous Environments

日時：2024年7月23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：金井 陽介

所属：ノースカロライナ大学チャペルヒル校

要旨：

The coupled quantum dynamics of electrons and protons is ubiquitous in many dynamical processes involving light-matter interaction including solar energy conversion in artificial photocatalytic devices and photosynthesis. A first-principles description of such nuclear-electronic quantum dynamics requires not only the time-dependent treatment of nonequilibrium electron dynamics but also that of quantum protons. We discuss new real-time nuclear-electronic orbital time-dependent density functional theory (RT-NEO-TDDFT) approach to study such dynamics in complex extended systems. We apply the new first-principles method to studying coupled quantum dynamics of electrons and protons in complex heterogeneous systems such as semiconductor-molecule interfaces and photoactive molecules in water. Developing the fundamental understanding for such quantum dynamical processes at the atomistic level is central to photocatalytic CO₂ reduction, as pursued in the U.S. Department of Energy's Energy Innovation Hub, Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) headquartered at the University of North Carolina at Chapel Hill (UNC). Our work articulates how atomistic environments such as hydrogen-bonding water molecules and an extended material surface impact the coupled quantum dynamical process. I will conclude by discussing outstanding challenges and other related method development efforts from my research group at UNC.

標題：行列積状態のゲージ自由度とその応用について

日時：日時：7月29日(月) 午前10時30分～午後4時45分 / 7月30日(火) 午前10時30分～午後4時45分

場所：東京大学 理学部1号館207号室 (本郷キャンパス)

講師：塩崎 謙

所属：京都大学 基礎物理学研究所

要旨：

概要： 行列積状態(MPS)とは、空間1次元系における量子状態の表現方法のひとつである。密度行列くりこみ群法(DMRG)など実用的な数値計算手法として重要なみならず、対称性によって保護されたトポロジカル相の数学的記述においても重要な役割を果たす。本講義では、MPSの数理物理学的な側面に焦点を当て、いくつか重要な帰結について議論したい。内容は以下を予定している。

antiferromagnetic (AFM) state through Bose-Einstein condensation. Duality in the power-law scaling of transition temperatures and an anomalous quantum critical scaling in the spin-lattice relaxation rates are revealed near the critical field. These results establish concrete experimental existence of a proximate DQCP, and provide a platform for further investigation of the properties of deconfined quantum criticality.

標題：Revealing unique light-matter interaction of the amplitude Higgs mode in superconductors by terahertz nonlinear spectroscopy

日時：2024 年 8 月 26 日(月) 午後 1 時～午後 3 時

場所：物性研究所本館 6 階 第 1 会議室 (A636) 及び Online (Hybrid)

講師：勝見 恒太

所属：New York University

要旨：

Light-matter interaction in quantum materials is a critical aspect that elucidate their intriguing properties. In particular, the terahertz (THz) frequency range is of great interest as it is the natural energy scale of quantum many-body interaction between charge, spin, orbital, and lattice degrees of freedom. Recent advancements in generating an intense THz pulse enabled the investigations of nonlinear light-matter interaction, which can provide information unreachable by linear light-matter coupling. However, the study of nonlinear light-matter interactions is still in its infancy, and experimental investigation is required.

Here, we will present the recent results of THz nonlinear spectroscopy applied to superconductors. Using THz two-dimensional coherent spectroscopy (2DCS), we identified a unique paramagnetic nonlinear response of the amplitude collective mode of the superconducting order parameter, namely the Higgs mode, in conventional superconductors NbN [1]. Our findings demonstrate the ability of THz 2DCS to explore collective excitations inaccessible in other spectroscopies. We will further discuss the results of THz 2DCS in the case of a multi-gap superconductor MgB₂. Finally, given the situation that the paramagnetic light-matter interaction plays an essential role in the THz nonlinearity in superconductors, we reexamine our previous THz pump-probe experiments in high-temperature cuprate superconductors Bi₂Sr₂CaCu₂O_{8+x} [2].

References:

[1] K. Katsumi et al., Phys. Rev. Lett. 132, 256903 (2024)

[2] K. Katsumi et al., Phys. Rev. Lett. 120, 117001 (2018)

標題：オープンアクセス実現に向けた研究データの公開戦略

日時：2024 年 8 月 29 日(木) 午後 4 時～午後 5 時

場所：物性研究所本館 6 階 A612 及び Online

講師：吉見 一慶

所属：物性研究所

要旨：

2024 年 2 月、内閣府は学術論文等の即時オープンアクセスの実現に向けた基本方針を提示した。この方針により、公的資金を受給する競争的研究費を対象に、該当する学術論文および根拠データの即時公開が義務付けられている。対象は 2025 年度から新たに公募を行う研究費である。これにより、多くの研究者や研究機関にとって、オープンアクセス化への対応が喫緊の課題となっているのではなかろうか。

本講演では、東京大学が運用する東京大学学術機関リポジトリ、物性研究所で 2021 年より運用している ISSP データリポジトリ、そして物質・材料機構の Materials Data Repository (MDR) など、いくつかのデータリポジトリを紹介する。さらに、これらのリポジトリを活用したオープンアクセス化の具体的な方法について提案する。これらの例を通じて、参加者全員と共にオープンアクセス化に向けた効果的なデータ管理方法について議論し、最適なアプローチを模索した。

53 物性研だより第64巻第3号

effect, which counterintuitively enhances the lifetime of the impurity against loss. We also find a crossover from the non-Hermitian Kondo regime to the valence fluctuation regime dominated by one-body dissipation. Our results can be tested in a wide variety of setups such as quantum dots coupled to electronic leads and quantum point contacts in ultracold Fermi gases.

[1] Kazuki Yamamoto, Masaya Nakagawa, and Norio Kawakami arXiv:2408.XXXXX to be submitted.

標題：Wave function geometry for bulk photovoltaics

日時：2024 年 9 月 11 日(水) 午前 10 時～

場所：物性研究所本館 6 階 第 5 セミナー室 (A615)

講師：Aris Alexandradinata

所属：University of California Santa Cruz

要旨：

Steady illumination of a non-centrosymmetric semiconductor results in a bulk photovoltaic current, which is contributed by real-space displacements (‘shifts’) of charged quasiparticles as they transit between Bloch states. The shift induced by interband excitation via absorption of photons has received the prevailing attention. However, this excitation-induced shift can be far outweighed (\ll) by the shift induced by intraband relaxation, or by the shift induced by radiative recombination of electron-hole pairs. This outweighing (\ll) is attributed to (i) time-reversal-symmetric, intraband Berry curvature, which results in an anomalous shift of quasiparticles as they scatter with phonons, as well as to (ii) topological singularities in the interband Berry phase (‘optical vortices’), which makes the photovoltaic current extraordinarily sensitive to the linear polarization vector of the light source. Both (i-ii) potentially lead to nonlinear conductivities of order mA/V^2 , without finetuning of the incident radiation frequency, band gap, or joint density of states. A case study of BiTeI showcases the anomalous shift and optical vorticity in a realistic material.

標題：Exact renormalization flow for Matrix Product Density Operators

日時：2024 年 9 月 30 日(月) 午後 3 時 30 分～午後 4 時 30 分

場所：物性研究所本館 6 階 第 5 セミナー室 (A615)

講師：加藤 晃太郎

所属：名古屋大学

要旨：

Matrix Product Density Operators (MPDOs) provide an efficient tensor-network representation of mixed states in one-dimensional quantum many-body systems, often used to describe thermal states and steady states in dissipative dynamics. While MPDOs generalize Matrix Product States (MPS), which effectively describe 1D pure states and are associated with gapped ground states, the renormalization properties of MPDOs are more complex. In this work, we investigate real-space renormalization group (RG) transformations of MPDOs, modeled as circuits of local quantum channels. We impose that the renormalization flow must exactly preserve correlations between coarse-grained sites, ensuring that it is invertible through other local quantum channels. We first show that unlike MPS, which always admit well-defined isometric renormalization flows, MPDOs generally do not exhibit such exact flows. We introduce a subclass of MPDOs with well-defined renormalization flows, showing that these states possess a coalgebra structure and obey generalized symmetries described by Matrix Product Operator (MPO) algebras. Additionally, we explore the fixed points of these renormalization flows, providing insights into the classification of mixed-state quantum phases and the role of non-invertible symmetries in this subclass of MPDOs.

標題：ハイスループット計算ツール moller の紹介

日時：2024 年 10 月 7 日(月) 午後 4 時～午後 5 時

場所：物性研究所 6階 A612 及び Online

講師：青山 龍美

所属：東京大学物性研究所

要旨：

mollerは、パラメータサーチなど一連の計算を網羅的に実行する際に、スーパーコンピュータやクラスター計算機を活用して一括計算(バルク実行)を行うための **Python** パッケージです。通常のジョブ実行スクリプトとほぼ同じ内容を記述したインプットファイルを用意して **moller**に入力すると、複数のジョブを **GNU Parallel**を利用して並列実行するジョブスクリプトが生成されます。現在は物性研スパコンに対応するほか、一般のワークステーションやクラスター計算機で利用できます。また、国内の主要なスーパーコンピュータシステムへの展開を計画しています。今回の物性アプリーオープンフォーラムでは、**moller**の機能や開発、**moller**を用いたハイスループット計算について紹介した。

標題：Specifics of spin excitations in centrosymmetric helimagnets

日時：2024年10月8日(火) 午後3時～午後4時

場所：物性研究所本館 6 階 第 2 セミナー室 (A612) 及び Online

講師：Dmytro Inosov

所属 : Neutron Spectroscopy of Condensed Matter, Technische Universität Dresden

要旨：

Noncollinear long-range ordered magnetic structures that break chiral symmetry can arise either as a result of Dzyaloshinskii-Moriya interactions in lattices with broken inversion symmetry or as a result of bond frustration in structurally centrosymmetric crystals. While in the former case the spin chirality is uniquely chosen by the lattice symmetry, in the latter case the chiral symmetry is broken spontaneously, so that both right- and left-handed magnetic domains can coexist. Using inelastic neutron scattering, we have studied spin waves in a number of centrosymmetric helimagnets with different magnetic ground states. The cubic spinel ZnCr_2Se_4 is described by frustrated interactions and represents a perfect model system for studying the Heisenberg model on the perfect pyrochlore lattice. Here, an emergent energy scale of the pseudo-Goldstone magnon gap leads to highly nontrivial thermodynamic and thermal transport properties and to the appearance of a field-induced spiral spin liquid state. The iron perovskite compounds SrFeO_3 and $\text{Sr}_3\text{Fe}_2\text{O}_7$, on the other hand, avoid the simple spin-spiral state and form multiple-q orders of various types, whose spin-wave spectrum is still a challenge for theoretical calculations. At elevated temperatures, all the mentioned compounds exhibit an intense quasielastic spin-fluctuation spectrum in neutron spectroscopy, which coexists with the sharp collective spin-wave excitations and could be a universal feature of the centrosymmetric helimagnets in general. It is possible that its origin is connected with the dynamics of domain walls that separate helimagnetic domains of opposite chirality.

標題：パルス強磁場・高圧力下磁化率測定プローブによる三角格子磁性体の圧力下磁場誘起相転移の研究

日時：2024 年 10 月 18 日(金) 午前 11 時～午後 0 時

場所：Online

講師：二本木 克旭 基礎科学特別研究員

所属：理化学研究所 創発物性科学研究センター 創発物性計測研究チーム

要旨：

強磁場・高圧力・極低温環境を同時に実現した複合極限環境は、電子のもつ内部自由度(スピン、電荷、軌道、格子)を直接変化させることで、新奇な物理現象の発現が期待できる。しかし、高い磁場を発生可能なパルス強磁場中では、速い磁場掃引速度によって圧力装置の金属部分に渦電流を発生させるため、電磁ノイズによる測定感度の低下やジュール発熱による試料温度の上昇といった技術的な問題がある。

阪大先端強磁場では、大型コンデンサバンクとミッドパルスマグネットによるパルス強磁場中で使用可能な金属製圧力セルの開発及び LC 共振回路における磁化率測定手法を導入した。その結果、最低温度 1.4 K において最大磁場 55 T、最高圧力 2.1 GPa で磁化率測定を実現[1]して、低温環境が必要な低次元磁性体の圧力下強磁場磁性を明らかにしてきた[2,3]。

本セミナーでは、三角格子磁性体 CsCuCl_3 および CsFeCl_3 の圧力下磁場誘起相転移の研究成果を基に本測定装置の現状及び今後の展開について報告した。

[1] K. Nihongi et al., Rev. Sci. Instrum. 94, 113903 (2023).

[2] K. Nihongi et al., Phys. Rev. B 105, 184416 (2022).

[3] K. Nihongi et al., J. Phys. Soc. Jpn. 93, 084704 (2024).

標題：Unveiling the Nexus Between Real and Momentum Space skyrmion in Correlated Systems

日時：2024 年 10 月 18 日(金) 午後 1 時 30 分～

場所：物性研究所本館 6 階 第 5 セミナー室 (A615)

講師：Dr. Shizeng Lin

所属：Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory

要旨：

In this talk, I will explore the emergent physics resulting from the complex interaction between real-space and momentum-space topology in strongly correlated quantum materials, with a particular focus on skyrmions. Using quantum Hall and quantum spin Hall insulators as key examples, I will explain the mechanisms behind skyrmion formation through electron doping in these correlated and gapped topological systems. We provide a detailed analysis of the phase diagrams and the formation of skyrmion lattices within the Kane-Mele-Hubbard model, supported by calculations from both the unrestricted real-space Hartree-Fock and density matrix renormalization group methods. In these systems, the doped electron and skyrmion form a composite object whose density is governed by the doped electron density. This electron-skyrmion bound state is stabilized by the coupling between the orbital magnetization of the Chern band and the emergent magnetic flux generated by the skyrmion. Moreover, we find that doping induces quantum anomalous Hall crystals, which exhibit quantized Hall conductance and broken translational symmetry. Our theory offers an intrinsic mechanism for the experimentally observed robust quantum anomalous Hall insulator over an extended doping range near a filling factor of $\nu = 1$ in twisted transition metal moiré superlattices.

Reference: Miguel Gonçalves and Shi-Zeng Lin, arXiv:2407.12198

