

# 物性研究

- [1] H. Nakamura et al., PRB 80, 121308 (2009).  
H. Nakamura et al., PRL 108, 206601 (2012).
- [2] S. P. Chiu et al., PRB 96, 085143 (2017).
- [3] H. Okuma et al., PRB 105, 045138 (2022).
- [4] H. Okuma et al., PRMater 8, 015001 (2024).
- [5] H. Okuma et al., arXiv:2403.12612.
- [6] H. Okuma et al., iWOE-29, Busan, Korea, P2-39, 15-18 Oct. 2023.

日時：2024 年 4 月 10 日(水) 午後 3 時～午後 4 時 30 分  
場所：物性研究所 6 階大講義室 及び Online (Hybrid)  
講師：林 悠偉

**要旨：**

SASデータ解析では、データに基づいて試料の構造情報を持つ散乱強度の数理モデルを仮定し、そのモデルのパラメータ推定を行う。従来の方法は簡便な一方で、しばしば属人的な結果が得られやすいことや、結果の信頼度評価が難しい等の課題がある。提案する枠組みは、SASデータ解析にベイズ推論の枠組みを応用し、パラメータやモデルを事後確率分布として推定することで従来法の課題を解決する。

本発表ではまず、一次モデル  $y=ax+b$  のパラメータのベイズ推定について説明する。ここで、パラメータの事後確率分布の統計量から推定の信頼度評価が可能であることを見る。次に、提案手法において SAS の試料モデルに適用するベイズモデル選択を、一次モデル  $y=ax+b$  と  $y=ax$  に適用しベイズモデル選択の理論を説明する。その後、様々なノイズ強度、欠損度合いの SAS 人工データを用いた数値実験を通して、試料パラメータ推定とモデル選択の提案手法の性能評価を行う。この結果から提案手法は、試料パラメータを信頼度付きで推定できる分布推定と、定量的で高精度な試料モデルの選択を可能とすることを示す。また、提案手法による解析の限界についての視座を提供した。

- Hayashi, Y., Katakami, S., Kuwamoto, S., Nagata, K., Mizumaki, M., & Okada, M. (2023). Journal of the Physical Society of Japan, 92(094002).
- Hayashi, Y., Katakami, S., Kuwamoto, S., Nagata, K., Mizumaki, M., & Okada, M. (2024, January). Quantitative selection of sample structures in small-angle scattering using Bayesian methods. Journal of Applied Crystallography. Manuscript submitted for publication. <https://arxiv.org/abs/2401.10466>

標題：Probability control nonreversible Markov chain Monte Carlo

日時：2024年4月11日(木) 午後1時～午後3時

場所：物性研究所本館 6 階 第 4 セミナ一室 (A614)

講師：Hidemaro Suwa

所属: Department of Physics, The University of Tokyo

**要旨：**

In recent developments, Monte Carlo methods that strategically break detailed balance to manipulate the flow of probabilities have emerged [1]. These methods include optimizing the transition probabilities during state updates. We developed an optimization algorithm designed to minimize the rejection probability and successfully applied it to various statistical mechanical models, such as the Potts model and quantum spin systems [2]. Further, we introduced an algorithm capable of controlling the rejection rate through a single parameter, revealing that reducing the rejection rate leads to an exponential increase in computational efficiency [3]. Another intriguing strategy for breaking detailed balance is the concept of lifting, which expands the state space to introduce probability flow in the enlarged state space. The lifting technique is particularly effective in particle systems, as demonstrated by the event chain Monte Carlo method [4]. In this talk, reviewing these approaches to constructing nonreversible Markov chains, we will present the lifted directed-worm algorithm [5,6] and the multi-replica swap optimization of the replica exchange method (namely, parallel tempering). These probability control nonreversible Markov chains significantly improve the computational efficiency of Monte Carlo sampling.

- [1] H. Suwa and S. Todo, Butsuri 77(11) 731-739 (2022).
- [2] H. Suwa and S. Todo, Phys. Rev. Lett. 105, 120603 (2010).
- [3] H. Suwa, Physica A 633, 129368 (2024).
- [4] W. Krauth, Front. Phys. 9:663457 (2021).
- [5] H. Suwa, Phys. Rev. E 103, 013308 (2021).
- [6] H. Suwa, Phys. Rev. E 106, 055306 (2022).

標題：Nanoscale 3D imaging through raster scan X-ray microscopy

日時：2024年4月22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：Zirui Gao

所属 : Brookhaven National Laboratory, New York, USA

**要旨：**

We have recently developed a novel raster-scanning based X-ray microscopy method at the Hard X-ray Nanoprobe (HXN) beamline of National Synchrotron Light Source II [1]. Our new method can achieve sub-10 nm resolution with acquisition speed  $\sim 20$  times faster than our previous approaches. The method utilizes ptychography in 2D fly-scan mode at an acquisition frame rate of 1250 diffraction patterns per second, currently limited by the fastest frame rate of the Eiger1 1M detector. By using ptychography, which is a coherent diffraction imaging method that reconstructs complex images of the sample through iterative phase retrieval algorithms [2], the sample image can be reconstructed at pixel size of 4.87 nm, providing imaging speed far beyond acquisition frame rate. As shown in Fig. 1(Left) is the reconstructed phase image of a Siemens star sample, our method can resolve the smallest features inside the pattern with 8 second of measurement time for a  $2\text{ }\mu\text{m} \times 2\text{ }\mu\text{m}$  field of view, effectively reaching an imaging speed of 23000 pixels per second.



Our new raster scan instrument also allows tomography measurement by acquiring 2D projections of the sample at different rotation angles. The sample stages and interferometry reference system are specially designed for precise rotation alignment with  $<0.5\ \mu\text{m}$  drift to minimize tomography acquisition overhead and increase imaging speed. As shown in Fig. 1(Right) is the reconstructed phase tomogram of a cylindrical-shaped microelectronics sample extracted from an Intel® processor, the entire tomography acquisition took 53 minutes in real time for an imaged region of  $2\ \mu\text{m}$  diameter and  $3\ \mu\text{m}$  height. The zoom-in view in Fig. 1(Right) shows the smallest resolvable feature in the tomogram which appears to be metallic connectors in transistors. In this talk, I will cover the key concepts and technical implementations of our novel imaging method.

**標題 :** Operator Growth in Open Quantum Systems : Perspectives from Lindbladian SYK via Krylov Complexity

**日時 :** 2024 年 4 月 24 日(水) 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 :** Budhaditya Bhattacharjee

**所属 :** Center for Theoretical Physics of Complex Systems, Institute for Basic Science

**要旨 :** Abstract:

In this talk, I will discuss some general features of operator growth in open quantum systems governed by Lindbladian evolution. I will introduce two orthonormalization techniques, namely Arnoldi and BiLanczos algorithms, using which I will capture the evolution of the operator in an appropriate basis. In these bases, many features of the evolution of operators (including relevant time scales) will emerge naturally. I will motivate these bases choices from results in closed quantum systems. I will utilize the paradigmatic setup of the Sachdev-Ye-Kitaev model to describe the system and environment, and closely related system-environment interaction. I will present numerical results in this setup and derive some analytical results. I will also discuss the nature of correlation function and spectral function in such open quantum systems. Then I will discuss features of a large class of probes (that do not rely on the same choice of basis) in such systems. I will end by mentioning implications of these results in other areas of research, and some open questions/future directions.

References:

[1] Operator dynamics in Lindbladian SYK: a Krylov complexity perspective, JHEP 01 (2024) 094

[2] Operator growth in open quantum systems: lessons from the dissipative SYK, JHEP 03 (2023) 054

**標題 :** Higher symmetry and logical gates of (3+1)D  $\mathbb{Z}_2$  toric code

**日時 :** 2024 年 4 月 25 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)および Online

**講師 :** 小林 良平

**所属 :** University of Maryland

**要旨 :**

It has recently been understood that the complete global symmetry of topological gauge theories contains the structure of a higher-group. In this talk, we look at the algebraic structure of symmetry in (3+1)D  $\mathbb{Z}_2$  gauge theory with an emergent fermion, and point out that pumping chiral  $p+i p$  topological states gives rise to a  $\mathbb{Z}_8$  0-form symmetry with mixed gravitational anomaly. This ordinary symmetry mixes with the other higher symmetries to form a 3-group



In this talk I would like to review how those interdisciplinary interactions has been developed from modern viewpoint, and also show the trend continues in the recent research.

**標題：多量体を形成する遷移金属酸化物の X 線光電子分光・吸収分光/ナノ構造物質からの高次高調波発生：バンド内遷移とバンド間遷移**

**日時：2024 年 5 月 20 日(月) 午後 1 時～午後 3 時**

**場所：物性研究所本館 6 階 第一会議室 (A636)&Online (ハイブリッド)**

**講師：大川 万里生 氏      中川 耕太郎 氏**

**所属：物性研究所 岡崎研究室      松永研究室**

**要旨：**

**(1) 講師：大川 万里生 氏**

題目：多量体を形成する遷移金属酸化物の X 線光電子分光・吸収分光

概要：

V 等の遷移金属酸化物では多量体形成により絶縁体相が安定化している例がしばしばみられる。光電子分光や X 線吸収分光は、物質の電子状態を直接反映したスペクトルが得られるため、遷移金属の多量体形成の検証に有用である。我々は、c 軸 Ti 二量体を形成するコランダム Ti<sub>2</sub>O<sub>3</sub> の Ti-Mg 置換効果を X 線吸収分光により、またパイロクロア格子中の W が三量体形成するとされる CsW<sub>2</sub>O<sub>6</sub> を X 線光電子分光により調べたので報告した。

[1] M. Okawa et al., PRB 108, 159108 (2023).

[2] R. Nakamura et al., PRB 106, 195104 (2022).

**(2) 講師：中川 耕太郎 氏**

題目：ナノ構造物質からの高次高調波発生：バンド内遷移とバンド間遷移

概要：

高次高調波発生 (HHG) はアト秒パルス発生や X 線光源などの応用に向けて注目される非線形光学現象である。近年では固体からの HHG が観測され[1]、特に電子のバンド内とバンド間での遷移によってその発生機構が理論的に議論されている。しかしながら、実験的にそれらの寄与を切り分ける研究は少ない。本講演では、ナノ物質であるナノ粒子とグラフェンに注目して、電子のバンド内遷移やバンド間遷移を制御し、HHG への寄与を解明した[2,3]。

[1] S. Ghimire et al., Nat. Phys. 7, 138 (2011).

[2] K. Nakagawa et al., Nat. Phys. 18, 874-878 (2022).

[3] K. Nakagawa et al., under review.

**標題：Stars in your eyes – monodisperse macromolecules for photonic and optoelectronic applications**

**日時：2024 年 5 月 27 日(月) 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. Peter J. Skabara**

**所属：School of Chemistry, University of Glasgow Glasgow, United Kingdom**

**要旨：**

We have developed a synthetic approach that allows us to synthesise monodisperse organic are semiconductor macromolecules on the gram scale. In contrast to conjugated polymers, batches are prepared with 100% reproducibility and the products can be isolated in high purity. These attributes are extremely well valued, because subsequent work

For the applications mentioned above, the materials have been designed to be amorphous with excellent film-forming properties and compatibility in composites. The latter includes hybrid LED devices and as wide band gap materials in optically transparent OPVs. This talk will highlight some of our recent work on the synthesis and application of star-shaped organic semiconductors [1-4].

- [1] H. Yang, P. J. Skabara et al., J. Mater. Chem. C, 2023, 11, 9984–9995.
- [2] M. Yan, P. J. Skabara et al., J. Mater. Chem. C, 2023, 11, 8480–8485.
- [3] K. Yoshida, P. J. Skabara et al., Nature 621, 746–752 (2023).
- [4] L. Lozano - Hernández a, P. J. Skabara et al., ChemPhotoChem. 2023, 7, e202200256.

**要旨：**

The comparative study reveals that bond-dependent anisotropic interactions, rather than isotropic Heisenberg interactions, amplify quantum entanglement, even in systems with geometrical frustration. The present study paves the way for the automatic design of new quantum systems with desired quantum nature and functionality.

**要旨：**

重力が物理を支配する極限天体の代名詞がブラックホールである。しかし、ブラックホール近傍で発生する多くの物理現象は、その磁気活動に起因していると考えられている。本セミナーでは、ブラックホール近傍での物理現象を概観しつつ、最新の理論・観測からわかってきたブラックホール近傍の磁気活動について紹介したい。