研究会報告 Stat&QuantPhys Autumn School 2021

開催日:2021年9月27日(月)・28日(火) 場所:オンライン(Zoomミーティング・oVice)

東京大学理学系研究科 山岸愛

研究の世界に足を踏み入れたばかりの学生にとって、同世代や先輩の研究者との交流は、研究 者としての視野を広げられる大切な機会となっていた。しかし、止まるところを知らない COVID-19の流行のために研究室の垣根を越えた交流の機会は以前に比べて希少なものとなって いる。Stat&QuantPhys Autumn School 2021 (SQP2021) は、このような状況に鑑みて有志の学生に より企画、開催された。

本スクールでは研究者や学生に幅広い交流の機会を提供することを目的とした。オンライン開催の利点を活かして留学生や海外の同年代の学生も参加できるよう、すべてのプログラムを英語で行うこととした。当日までに日本を含む15カ国から270名の参加登録があり、狙い通り諸外国の学生や研究者、留学生にも多数参加いただくことができた。当日は6名の招待講演者による講義と15名の参加者によるポスター発表が行われ、大いに盛り上がった。

参加者や運営委員にとって英語開催はハードルが高くなることを危惧していたが(そして実際 に参加者や講師への連絡等を毎度英作文するのは非常に骨の折れる作業であったが)、蓋を開けて みると、日本語のみでのコミュニケーションでは知り合うことのなかった人々が本スクールを通 じて知り合う場面を目にすることもあり、多くの参加者にとって有意義な機会になったと自負し ている。筆者自身も、一参加者として講義中やポスターセッションにおける活発な議論を大いに 楽しんだ。また、ポスター発表も行い、他の参加者と知り合ったのみならず、自身のモデルを再 考する契機を得ることもできた。

<u>プログラム</u>

本スクールは表1のプログラムで開催した。時間は日本時間による表記である。開校式と各講 義、ポスター発表にはZoomミーティングを用いた。講義ではSlidoというツールも併用し、専門 用語の対訳を書き込むなどして参加者の理解を助けるよう工夫した。また、開催期間中は oVice を用いたバーチャルプラットフォームを提供して参加者が自由に交流できるようにし、懇親会で はその会場を活用した。詳細はウェブサイト[1]に掲載されている。

	9/27 Mon.	9/28 Tue.
8:45-9:00	Opening ceremony	
9:00-12:00	Lecture 1 / Lecture 2	Lecture 3 / Lecture 4
12:00-13:00	Lunch-time chat	Lunch-time chat
13:00-16:00	Poster presentations	Lecture 5 / Lecture 6
16:00-	Get-together	Get-together

表 1: Stat&QuantPhys Autumn School 2021 の全体プログラム

[1] SQP2021 ウェブサイト: <u>http://hatano-lab.iis.u-tokyo.ac.jp/yoshi9d/QSP2021/Index.html</u>

◯講義

6名の招待講演者と各講義のタイトルは以下の通りである。講義のアブストラクトを本稿の末 尾に掲載する。

- Lecture 1: Prof. Tomotoshi Nishino (Kobe University) "Tensor Network Formulation - Basic Concepts and Applications -"
- Lecture 2: Prof. Ko Okumura (Ochanomizu University) "Critical phenomena and scaling: from bubble breakup to kirigami mechanics"
- Lecture 3: Prof. Takahiro Sagawa (The University of Tokyo) "Thermodynamics of information: An introduction"
- Lecture 4: Dr. Kazuaki Takasan (University of California, Berkeley) "Nonequilibrium phases of matter: An introduction and recent developments"
- Lecture 5: Dr. Neill Lambert (RIKEN) "Open Quantum Systems: from qubits to quantum biology"
- Lecture 6: Dr. Takashi Mori (RIKEN) "Introduction to some basic notions of modern machine learning"

○ポスター発表

ポスター発表者と各発表のタイトルは以下の通りである。

- ・A-1: Tomohiro Soejima (University of California, Berkeley) ★ポスター賞受賞 "DMRG simulation of twisted bilayer graphene"
- A-2: Ken Mochizuki (Tohoku University)
 "Fate of topological edge states in periodically driven nonlinear systems"
- A-3: Daisuke Shimamoto (The University of Tokyo)

"Structure of the quasi-self-similar particle packing"

• A-4: Miku Ishizaki (The University of Tokyo)

"Non-Markovian Dynamics of Quantum Otto Cycle and analysis of work extraction"

• A-5: Takuya Furusawa (Tokyo Institute of Technology)

"Anomaly-induced edge currents in hydrodynamics with parity anomaly"

- A-6: Tianpu Zhao (Northwestern University)
 - "AB INITIO DEVELOPMENT OF GENERALIZED LENNARD-JONES (MIE) FORCE FIELDS FOR PREDICTIONS OF THERMODYNAMIC PROPERTIES IN ADVANCED MOLECULAR-BASED SAFT EQUATIONS OF STATE"
- A-7: Hongchao Li (The University of Tokyo) "Quantum Kinetic Theory of Nonlinear Response"
- B-1: Juan Pablo Bayona Pena (Tokyo Institute of Technology)
 "Thermodynamics of a continuous quantum heat engine: Interplay between population and coherence"
- B-2: Takato Mori (The Graduate University for Advanced Studies (SOKENDAI))

"Entanglement entropy in interacting quantum field theories"

• B-3: Yusuke Nakai (YITP)

"The construction of a topological number that can characterize skin effects in disordered onedimensional systems"

- B-4: Keisuke Matsumoto (Tokyo University of Science) "Introduction to Stochastic Resonance"
- B-5: Manami Yamagishi (The University of Tokyo)

"Defining a quantum active Brownian particle using a PT symmetric quantum walk"

• B-6: Kazuki Sone (The University of Tokyo)

"Topological synchronization of coupled nonlinear oscillators"

• B-7: Yuji Maruyama (Waseda University)

"Rotation of chiral liquid crystals driven by a temperature gradient"

• B-8: Atsuki Yoshinaga (The University of Tokyo)

"Hilbert Space Fragmentation in the two-dimensional Ising model with a weak transverse field"

謝辞

6 名の招待講演者の皆様におかれましては、基礎事項のおさらいから最近の研究の話題まで丁 寧に解説していただきました。特に、英語で、しかも限られた時間のなかで幅広い分野の学生向 けの入門的講義をするというお願いを快く引き受けて下さり、深く感謝申し上げます。また、ポ スター発表いただいた皆様には興味深い発表にお礼申し上げます。そして、ポスター発表や講義 を盛り上げて下さったすべての参加者、開催にあたり格別のご協力を賜りました東京大学羽田野 研究室、早稲田大学山崎研究室に深く感謝の意を表します。

最後に、運営委員会の立ち上げからスクール当日まで非常に短い期間であったにも関わらず前 向きな姿勢で万端に準備を進めて下さった運営委員の皆様、本当にありがとうございました。

運営委員

高靜儀(東大、羽田野研 M1) 石崎未来(東大、羽田野研 D1) 王鑫(東大、羽田野研 M1) 上村俊介(筑波大、都倉・吉田研 D1) 多賀圭理(早稲田大、山崎研 D2) 松本佳大(東京理科大、二国研 M1) 山岸愛(東大、羽田野研 M1)(代表) 吉田大希(東大、山下研 M1) 吉永敦紀(東大、羽田野研 D2)

Tensor Network Formulation - Basic Concepts and Applications -

Tomotoshi Nishino (Kobe University)

Tensor network (TN) formulation has been applied to a variety of problems in statistical and quantum physics. In this lecture we start from the basic concepts and elementary structure of TN. In particular, we focus on the matrix product (MP), which satisfies important aspects of TN, which are the representability of a wide class of states and the computability in the applications to practical problems. It should be noted that a large portion of states we consider in physics, such as low-energy states and thermal equilibrium states, are less entangled. This physical property enables us to precisely approximate, or sometimes exactly represent, those states under consideration. The TN study starts from believing in such a representability, although it should be verified afterward; the state you'd like to analyze can be expressed by TN.

The TN is constructed by means of contracting tensors. Thus there are so many adjustable parameters, and this is the reason why TN has a high potential of approximating a wide class of states. On the other hand, there are two many parameters to be optimized, and therefore computational treatment is avoidable in the TN formulation. There are several numerical algorithms for this purpose. The density matrix renormalization group (DMRG) is a well known example, which optimizes the MP part by part successively. The numerical processes in DMRG can be naturally understood from the variational principle with respect to the MP state (MPS). Within a limited time, let us glance at other representative algorithms, such as corner-transfer matrix (CTM) formalism, time evolving block decimation (TEBD) scheme, multiscale entanglement renormalization Ansatz (MERA), etc.

Probably we have some time to see applications of TN formalism to correlated systems. A big progress has been achieved by the TN renormalization (TNR), where the flow toward the fixed point in renormalization group (RG) is correctly captured. I conjecture that, some time in far (?) future, a sort of layered TN enables us to express a macroscopic system that contains classical information, from the view point of quantum mechanics in microscopic world.

References

 Please access the following web page to capture the daily developments in this field: http://quattro.phys.sci.kobeu.ac.jp/dmrg/condmat.html

Critical phenomena and scaling: from bubble breakup to kirigami mechanics

Ko Okumura

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Critical phenomena in statistical physics are mathematically singular behaviors of physical quantities as a function of thermodynamic variable at a critical point. Near the critical point, the singular behaviors are characterized by scaling laws. Although the critical point is non-universal, the scaling exponents are universal for any materials (or models) if they are in the same universality class. Understanding of physical or mathematical mechanism for the emergence of universality was one of the central topics in physics in 1960's and, currently, is a highlight in the master course in physics.

P. G. de Gennes noticed a deep analogy of this thermodynamic problem with scaling that appears in polymer physics, after he understood a preprint written by K.G. Willson. As a result, two papers, one by Willson and the other by de Gennes were published on February 28, 1972. This day revolutionized physics, specifically, the history of statistical physics and that of polymer physics, at the same time, leading to two separate Nobel prizes in 1985 and 1991.

In the first part of the lecture, we give a brief overview on physical understanding of critical phenomena and its relation to polymer physics. In the second part, we give two more analogies with the thermodynamic problem [1]. One is associated with the dynamics of bubble breakup, a topological transition of the shape [2]. The other appears in a mechanical transition when kirigami, a paper with cuts of a certain pattern, is extended [3]. We hope the audience will enjoy analogy in physics, from the three examples, which are all seemingly quite different but share common features!

[1] 奥村 剛、「印象派物理学入門」、214頁、日本評論社(2020年)

[2] Hana Nakazato, Yuki Yamagishi, and Ko Okumura, Self-similar dynamics of air film entrained by a solid disk in confined space: A simple prototype of topological transitions, Phys. Rev. Fluids 3, 054004 (2018)

[3] Midori Isobe and Ko Okumura, Continuity and discontinuity of kirigami's highextensibility transition: a statistical-physics viewpoint, Phys. Rev. Research 1, 022001(R)(2019)

Thermodynamics of information: An introduction

Takahiro Sagawa

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In the nineteenth century, J. C. Maxwell considered a hypothetical being that can observe and manipulate individual atoms and molecules, which leads to the apparent violation of the second law of thermodynamics. Such a being was named Maxwell's demon and has been an issue of intense controversies from the viewpoint of the foundation of thermodynamics. Nowadays, it is realized that information is the key concept to understand the consistency between the demon and the second law.

In this decade, thermodynamics of information has attracted renewed attention in light of modern nonequilibrium statistical mechanics, both theoretically and experimentally (see [1] for a review article). Theoretically, a general formulation of the second law has been established, where information contents, such as Shannon information and mutual information, and thermodynamic quantities, such as work and heat, are treated on an equal footing. Experimentally, Maxwell's demon has been realized by real experiments with various systems in both the classical and quantum regimes.

In this lecture, I will talk about a general theory of thermodynamics of information, starting from a brief introduction to nonequilibrium statistical mechanics and information theory. Specifically, I will focus on the generalization of the second law and the fluctuation theorem by incorporating information contents, leading to a general resolution of the paradox of Maxwell's demon. I will also talk about experimental realizations of Maxwell's demon by using colloidal particles and single electrons. Moreover, I will talk about a more advanced framework of thermodynamics for autonomous information processing, such as biochemical information processing, where continuous information flow plays a significant role.

[1] J. M. R. Parrondo, J. M. Horowitz, T. Sagawa, Nature Physics 11, 131-139 (2015).

Nonequilibrium phases of matter: An introduction and recent developments

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In the past decade, the development of experimental techniques has made it possible to realize and observe nonequilibrium states in many-body quantum systems, including solid-state systems and atomic-molecular-optical (AMO) systems. Theoretical researches have also been stimulated by this development and nonequilibrium quantum phenomena have become an important research subject in condensed matter physics in recent years. Using such nonequilibrium phenomena, it has become possible to realize quantum phases far away from equilibrium as steady or metastable states. Here, we call such states *nonequilibrium phases of matter*. They are not contained in the equilibrium phase diagram and are considered to be a new frontier, where exotic phases difficult to be realized in equilibrium (e.g., room temperature superconductivity) can be realized. In this lecture, I will start with an overview of the nonequilibrium phases of matter. I will present the background of the developments and what kinds of phases have been gathering interests in recent years.

Then, among the nonequilibrium phases of matter, I will focus on *Floquet systems* and *non-Hermitian systems* in this lecture. In Floquet (periodically driven) systems, the approach called Floquet engineering has been proposed to realize the desired quantum state by choosing an external drive and has been actively studied both theoretically and experimentally [1]. In particular, related experiments in solids driven by strong laser light are still challenging and gathering great attention recently [2]. In this lecture, I will explain the idea of the Floquet engineering for photoinduced phase transitions in solids, and then introduce several basic theoretical examples and corresponding experiments. If time allows, I will explain our works in this direction [3]. Non-Hermitian systems have attracted renewed attention in recent years thanks to the developments in the AMO experiments [4]. Since the recent developments are too rapid to be covered in this lecture, I will focus on asymmetric hopping models, which is the simplest example of the non-Hermitian topological phases [5]. Also, I will explain the related projects, where we introduced a model similar to the asymmetric hopping model and showed that the model can be regarded as a quantum analog of active matter [6].

- [2] J. W. McIver, et al., Nat. Phys. 16, 38-41 (2020).
- [3] KT, A. Daido, N. Kawakami, Y. Yanase, Phys. Rev. B 95, 134508 (2017).
- [4] Y. Ashida, Z. Gong, M. Ueda, Adv. Phys. 69, 3 (2020).
- [5] Z. Gong, Y. Ashida, K. Kawabata, <u>KT</u>, S. Higashikawa, M. Ueda, Phys. Rev. X 8, 031079 (2018).
- [6] K. Adachi, KT, K. Kawaguchi, arXiv:2008.00996.

^[1] T. Oka and S. Kitamura, Annu. Rev. Condens. Mat. Phys. 10, 387-408 (2019).

"Open Quantum Systems: from qubits to quantum biology"

Neill Lambert

Theoretical Quantum Physics Laboratory, RIKEN Cluster for Pioneering Research, Wako-shi, Saitama 351-0198, Japan

In this talk I will discuss the role of noise in both quantum technologies and quantum biology. I will begin with an introduction to how noise is treated within quantum mechanics, and how we can obtain open-system dissipative models by including an environment in the closed system model and tracing it out. I will then discuss the importance of such models through practical examples in QuTiP [1], our open-source library, with a focus on how to model Noisy Intermediate Scale Quantum Technologies and quantum circuits.

I will then give an overview of why many of the same models can be used to study examples in quantum biology, including photosynthesis and avian magnetoreception. Finally, I will show what happens when the approximations in these approaches break down, and we must move to more sophisticated "non-Markovian" methods [3], where the environment begins to regain quantum features that we had earlier discarded.

[1] <u>www.qutip.org</u>

[2] Scholes, G., Fleming, G., Chen, L. *et al.* Using coherence to enhance function in chemical and biophysical systems. *Nature* **543**, 647–656 (2017). Lambert, N., Chen, YN., Cheng, YC. *et al.* Quantum biology. *Nature Phys* **9**, 10–18 (2013).

[3] Lambert, N., Ahmed, S., Cirio, M. *et al.* Modelling the ultra-strongly coupled spin-boson model with unphysical modes. *Nat Commun* **10**, 3721 (2019).

Introduction to some basic notions of modern machine learning Takashi Mori

RIKEN Center for Emergent Matter Science (CEMS)

Deep learning has achieved unparalleled success in various applications such as image classification, speech recognition, natural language processing, and natural science. Remarkably, in modern machine learning applications, impressive generalization performance has been observed in an *overparameterized* regime, in which the number of trainable parameters of the network greatly exceeds the number of training data samples. Theoretically, it is recognized that the generalization error shows the so called double-descent curve: the generalization error first increases but at a certain threshold starts to decrease as the number of parameters increases. It is surprising because what we have learned in traditional statistical learning theory is that such an overparameterized network exhibits poor generalization due to overfitting to the training data. To understand the success of modern machine learning, a new theoretical framework would be demanded.

My lecture consists of two parts. In the first part, I first try to give an overview of theoretical studies of modern machine learning, including my own attempts [1, 2], with emphasis on physics perspective. I will explain double-descent curve and its implications, benefits of depth of neural networks [1], and Langevin dynamics approach to learning dynamics [2].

In the second part, I show you an analytical derivation of the double-descent curve in a simple linear regression problem. I will make a brief comment on what happens in more involved situations which are relevant to modern machine learning applications.

[1] Takashi Mori and Masahito Ueda, "Is deeper better? It depends on locality of relevant features", arXiv:2005.12488

[2] Takashi Mori, Liu Ziyin, Kangqiao Liu, and Masahito Ueda, "Logarithmic landscape and power-law escape rate of SGD", arXiv:2105.09557.