NATIONAL
CENTER *for*
THEORETICAL
SCIENCES
Physics Division
國家理論科學研究中心
物理組

2023-2024 NCTS PHYSICS
Biannual Report

2023-2024 NCTS Physics Biannual Report

Photo Credit 蔡岳倫

National Center for Theoretical Sciences (Physics Division)

國家理論科學研究中心（物理組）

October 2024

Contents

Publisher
Prof. Guang-Yu Guo

Editors
Ms. Chao-Jung Kuo, Ms. Jhan Yu Chen, Ms. Yu-Rou Tsang

Preface

The first half of the fifth phase (i.e., Phase V-I) of the National Center for Theoretical Sciences (NCTS) started in January 2021 and will operate until December 2025. This is the fourth year and this is the second Biannual Report. Also, National Science and Technology Council (NSTC) will conduct a review of the NCTS by the end of this year.

First of all, we held the first meeting of the International Advisory Committee (IAC) on June 20-21 last year. We are fortunate that five IAC members (Profs. Eberhard K. U. Gross, Jean-Francois Joanny, Kimyeong Lee, Chung-Pei Ma and Naoto Nagaosa) were able to participate the IAC meeting (see Photo 1). During the two-day meeting, the IAC members worked diligently and efficiently. They listened to the opening address by NTU Executive Vice President Wanjiun Liao, reports from the Director and Thematic Group (TG) Coordinators, talked to Executive Committee (EC) Members, Center Scientists and Center Postdocs, and also toured the Center viewing the Center facilities. The IAC members have provided us with very helped comments and suggestions to improve the Division to a higher level of excellence (More details on this event, including the report of recommendations by the IAC, are given in Sec. IV). We have been working on implementing these IAC recommendations since then. For example, to provide more opportunities for exchange and collaboration within the NCTS Physics as well as with the wide physics community, we initiated the annual NCTS Physics Winter and Summer Colloquiums last winter.

Photo 1: Photo taken just before the first session of the IAC Meeting.

In the past two years, NCTS Physics has significantly advanced theoretical physics research in Taiwan. Members of NCTS Physics have made outstanding contributions in areas from quantum computing and quantum information science, high energy physics and quantum field theory, theory and computational astrophysics, to condensed matter physics and quantum materials as well as chemical physics, nanoscience and complex systems, as presented in this Biannual Report. NCTS Physics published 161 papers in 2023, and has also published 137 papers so far this year. The publications are mostly of high academic quality with highly impactful results appearing in prestigious journals such as Science and Nature (see Sec. I.B). In particular, 31 and 33 papers were published in journals with top 15% of impact in 2023 and 2024, respectively. We notice that compared with other theoretical physics centers and institutions in the world such as Asian Pacific Center for Theoretical Physics (APCTP), the academic achievements of the Division appear rather outstanding.

Academic achievements of NCTS Physics members have been recognized by various national and international honors and awards in the past two years. Among young NCTS Physics members, in particular, Min-Kai Lin (CS) won the 10th FAOS Young Scholars' Creativity Award. Hsiang-Yi Yang (CS) received 2023 NSTC Ta-You Wu Memorial Award. Among senior NCTS Physics members, for example, Ray-Kuang Lee (CS) became an elected Optica Fellow. Yeong-Cherng Liang (CS) won 2024 Paul Ehrenfest Best Paper Award for Quantum Foundations. Yu-tin Huang was elected Fellow of TPS. Horng-Tay Jeng (CM), Chao-Ping Hsu (CS) and Ray-Kuang Lee received 2023 NSTC Outstanding Research Award. Pei-Ming Ho (CM) won MOE 67th Academic Award, and Guang-Yu Guo (CM) won MOE 27th National Chair Professor.

Photo 2: The inaugural NCTS-iTHEMS (RIKEN) Joint Workshop, August 2024.

NCTS Physics has actively promoted interaction and collaboration both within the domestic physics community and with researchers overseas in recent two years. We organized about 25 workshops and conferences in 2023. Among them, nine were joint meetings with foreign countries. We have held around 13 workshops and conferences so far this year. Of which, seven were joint meetings with other countries. We have hosted 224 and 134 foreign visitors in 2023 and 2024, respectively.

In the past two years, we have encouraged academic exchanges and collaborations between different disciplines, with domestic and overseas institutions, as well as with industrial R&D centers. For example, we organized an “NCTS Phys-Math Joint Summer School on Quantum Information Science” with Mathematics Division each year. Also, an MOU with the iTHEMS of RIKEN, Japan was signed in December 2022, and thus NCTS Physics organized the first NCTS-iTHEMS Joint Workshop titled “from Matters to Spacetime: Symmetry and Geometry” in August this year (see Photo 2). Finally, NCTS Physics organized a Theoretical Physics Forum in the Annual Meeting of Taiwan Physical Society each year to interact with the broad physics community.

An important part of NCTS Physics efforts has been the cultivation and nurturing of young scientists. To transfer the frontier research to the next generations, we organized eight and seven advanced schools in 2023 and 2024, respectively. To encourage young scholars to engage in theoretical physics research and to foster outstanding talents, NCTS Physics organizes three NCTS Awards each year, namely, the Young Theorist Award, Postdoc Best Paper Award and Student Outstanding Paper Award.

Finally, please look over the rest of this report which details the activities and achievements of NCTS Physics from January 2023 to October 2024. We would appreciate your continuing support and advice for the Division, which are important for its success.

Guang-Yu Guo 郭光宇

Director, Physics Division, NCTS
October 2024

I. Report of the Division Director

A. Overview

A.1 Physics Division of The NCTS

The National Center for Theoretical Sciences (NCTS) was established in August 1997 by the National Science Council [NSC, which had become Ministry of Science and Technology (MOST) from March 2014 to July 2022, and has become National Science and Technology Council (NSTC) since July 2022], with strong endorsement from some of the most eminent scholars, including Professors Chen Ning Yang and Shing-Tung Yau. It is currently located on the campus of National Taiwan University (NTU), Taipei, with NTU acting the host. The Center consists of two divisions: Mathematics and Physics Divisions.

NCTS was initially hosted by National Tsing Hua University (NTHU), Hsinchu, with NTHU and the adjacent National Chiao Tung University acted as co-host from 1997 to 2014. In response to the need of the community, sub-projects at NTU and National Cheng Kung University (NCKU) were added to the operation during 2002-2014. This arrangement of NCTS, together with the implementation of the Focus Group Program has greatly broadened and strengthened the interaction and collaboration among domestic scientists, which were the medium-term goals set up for that period of time.

In 2013, an international review on NCTS was conducted and it was concluded to be of high importance for NCTS to play a more prominent international role. A restructuring of the Center, including the abolishment of sub-projects together with a significant increase in funding was recommended, with the goal to promote NCTS to become an international leading academic center. It was also decided that Physics and Mathematics Divisions do not need to be hosted by the same university. As a result, a national call competition was made in the beginning of 2014. NTHU won the bid to operate Physics Division of NCTS. Mathematics division was hosted by NTU. The two divisions operate separately to serve their separate communities and cooperate on some of their national programs.

In 2020, another national call competition for Phase V NCTS was made. NTU won the bid to operate Physics Division as well, and consequently hosts both Mathematics and Physics Divisions since January, 2021. To increase the efficiency of the operations, Physics Division sets up NCTS Hubs in Hsinchu and southern part of Taiwan. Currently, there are four NCTS Hubs located on the campuses of NTHU, National Yang Ming Chiao Tung University (NYCU), NCKU and National Sun Yat-sen University (NSYSU).

Missions and Goals:

NCTS has the dual goal of becoming a center of excellence and a platform to serve the whole community. Specifically, the aim of the NCTS can be summarized as the following four missions or goals (Fig. A1.1): (1) To become a center of excellence in theoretical sciences and attract young researchers to do the frontier research, (2) To cultivate world class researchers and empower talented students, (3) To serve all theoretical scientists in Taiwan and foster interdisciplinary research, and (4) To promote international cooperation and collaborations.

Fig. A1.1 The four goals of the NCTS.

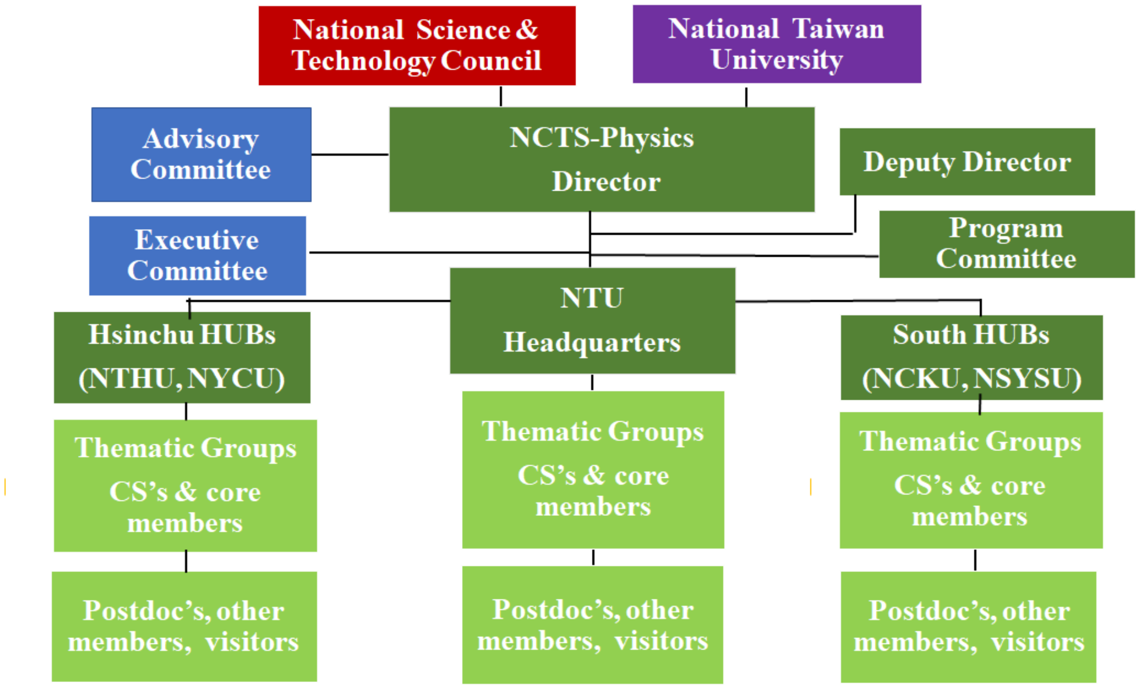


Fig. A1.2 Organization structure of Phase V NCTS Physics Division.

Organizational Framework:

To better achieve the four missions of the NCTS, the organization structure and major programs of Phase V NCTS Physics Division feature (1) one center augmented with four hubs, and (2) thematic group (TG) program (Fig. A1.2), as outlined in the 2020 NTU proposal for NCTS Physics. First, in order to serve the whole theoretical physics community and to increase the efficiency of the operations, NCTS Physics Division has set up four NCTS Hubs in the middle and southern part of Taiwan by the geographical distribution of the center scientists and members of the TGs. Second, to efficiently become a center of excellence, to better promote collaboration and to train our young researchers, the Physics Division has set eleven Thematic Groups (see Table A1.5 below) which combine the Distinguished Center Scientist (DCS) and Thematic Group Programs in the previous phase of the NCTS Physics (see Sec. A2 below)

Operation and Management:
Director is responsible for all the decisions of the Physics Division. Deputy Director assists the Director in implementing policies and operations of the Division. Director chairs the Executive Committee (EC). The EC consists of Director, Deputy Director, physics panel conveners from NSTC and several well-respected representatives from institutions over Taiwan appointed by NSTC NCTS Review Panel. EC members meet about once every three months, to discuss important issues related the Center, including the selection and evaluation of the Thematic Groups (TGs, see section A2), budgeting, approval of the Center Scientists (CSs), major changes of the plans and budgets as well as the general policies and guidelines for the NCTS scientific activities. (see Table A1.1 for the current EC members).

Table A1.1: Executive Committee (EC) members.

Name of EC member	Institution	Capacity
Guang-Yu Guo	National Taiwan University	Director
Jeng-Da Chai	National Taiwan University	Deputy Director
Jinn-Kong Sheu	National Cheng Kung University	Panel Convener
Wei-Hao Wang	Institute of Astronomy, Academia Sinica	Panel Convener
Hsiang-Kuang Chang	National Tsing Hua University	
Yueh-Nan Chen	National Cheng Kung University	
Chon-Saar Chu	National Yang-Ming Chao-Tung Univ.	
You-Hua Chu	Institute of Astronomy, Academia Sinica	
Pei-Ming Ho	National Taiwan University	
Henry Tsz King Wong	Institute of Physics, Academia Sinica	

Table A1.2: Program Committee (PC) members.

Name of PC member	Institution	Capacity
Guang-Yu Guo	National Taiwan University	Director
Jeng-Da Chai	National Taiwan University	Deputy Director
Hsi-Sheng Goan	National Taiwan University	TG1.1 Coordinator
Wen-Te Liao	National Central University	TG1.2 Coordinator
Hong-Bin Chen	National Cheng Kung University	TG1.3 Coordinator
Cheng-Wei Chiang	National Taiwan University	TG2.1 Coordinator
Yu-tin Huang	National Taiwan University	TG2.2 Coordinator
Min-Kai Lin	Academia Sinica	TG2.3 Coordinator
Feng-Chuan Chuang	National Sun Yat-sen University	TG3.1 Coordinator
Chung-Hou Chung	National Yang Ming Chiao Tung Univ.	TG3.2 Coordinator
Pochung Chen	National Tsing Hua University	TG4.1 Coordinator
Liang-Yan Hsu	Academia Sinica	TG4.2 Coordinator
Pik-Yin Lai	National Central University	TG4.3 Coordinator

Program Committee (PC) is comprised of the coordinators of the Thematic Groups (see section A1.2 below) as well as the Director and the Deputy Director (see Table A1.2 and also the Center's webpage). The PC holds a meeting each month chaired by the Director, discussing Center's operational matters such as postdoc hiring, coordinating inter-TG activities, monitoring TG's academic activities and budget expenditure etc.

The divisional routine and daily operations are carried out by the center administrative team which currently consists of four members of the administrative staff at the Center (NTU) as well as five administrative assistants in its Hubs in Hsinchu, Tainan and Kaohsiung (see Table A1.3).

Table A1.3: Current administrative assistants (https://phys.ncts.ntu.edu.tw/en/people/member4).

Name of assistant	Location	Role
Chao-Jung Kuo	Center (NTU)	Manager, Personnel, Accounting
Jhan Yu Chen	Center (NTU)	Personnel, TG 1.1, TG 4.1
Chia Chi Lin / Mu-I Liang	Center (NTU)	Space, TG 2.1, TG 2.3, TG 4.3
Yu-Rou Tsang / Nicole Wang	Center (NTU)	Accounting, TG 2.2, TG 4.2
Jia-Yi Hsu	Hsinchu Hub (NTHU)	Personnel, Accounting, TG 1.2
Renee Ho	Hsinchu Hub (NTHU)	Accounting, TG 4.1, TG 4.2
Ming Chuan Tsai	Hsinchu Hub (NYCU)	Accounting, TG 3.2, TG 4.3
Yi-Wen Fu	Tainan Hub (NCKU)	Accounting, TG 1.3, TG 3.1
Yu-Ping Chuang	Kaohsiung Hub (NSYSU)	Accounting, TG 2.2, TG 3.1

The Division also set up an International Advisory Committee in 2022 to aid it at the advisory level. Seven world renowned scientists accepted our invitations to serve in the IAC (see Table A1.4) and they would meet once every 2 years. The main function is to advise the Director on scientific priorities and to provide general guidance on the direction and development of the NCTS.

Table A1.4: International Advisory Committee (IAC) members.

Name of IAC member	Institution	Fields of expertise
Eberhard K. U. Gross	Hebrew Univ. of Jerusalem	Molecular & condensed matter theory
Jean-Francois Joanny	PSL Research Univ.	Complex systems
Kimyeong Lee	Korea Inst. for Advanced Study	Quantum field theory
Chung-Pei Ma	Univ. of California, Berkeley	Astrophysics
Naoto Nagaosa	University of Tokyo	Condensed matter theory
Franco Nori	RIKEN	Quantum comp. & information science
Carlos E. M. Wagner	University of Chicago	High energy physics

A.2 Summary of Academic Programs

Thematic Groups Program:

In Phase V, the main strategy of Physics Division to achieve the four goals of the NCTS (Fig. A1.1) is to build and serve the international competitive teams called Thematic Groups (TGs). In Jan., 2021, eleven such TGs in four grand fields (see Table A1.5) were organized by the Division and approved by the EC. They are identified based on the two considerations: namely, (1) teams in Taiwan that are internationally competitive in fields that are important in the coming decade and (2) fields that are important for the next decade and Taiwan have the potential to do well with sufficient support or cannot afford to be left out. The Thematic Groups are run by their respective center scientists (CSs) and core members. They have been provided with an ample research funding (about 4M for each TG on average) that can be used for the appointment of postdoctoral researchers as well as organizing activities such as conferences, schools and hands-on courses etc. Indeed, more than 90 % useable budget of the Division has been channeled to the TGs operations. Also, the four grand TGs are introduced in order to encourage and enhance the collaborative and innovative atmosphere of the larger community. The TGs and CSs are reviewed every two years. Thus, the current 11 TGs (Table A1.5) were reviewed and approved by the EC at the end of 2022.

Table A1.5: List of Thematic Groups (https://phys.ncts.ntu.edu.tw/en/program/page400).

	Thematic group	Coordinator
TG 1	Quantum Information and Quantum Computing	
TG 1.1	Quantum computing and interdisciplinary applications	Hsi-Sheng Goan
TG 1.2	Quantum physics and engineering	Wen-Te Liao
TG 1.3	Quantum information and communications	Hong-Bin Chen
TG 2	High Energy Physics and Astrophysics	
TG 2.1	High energy phenomenology	Cheng-Wei Chiang
TG 2.2	High energy theory	Yu-tin Huang
TG 2.3	Theoretical and computational astrophysics	Min-Kai Lin
TG 3	Condensed Matter and Materials Physics	
TG 3.1	Computational quantum materials	Feng-Chuan Chuang
TG 3.2	Strongly correlated condensed matter and cold atom systems	Chung-Hou Chung
TG 4	Interdisciplinary Research	
TG 4.1	High-performance computation and machine learning	Pochung Chen
TG 4.2	Chemical physics, physical chemistry and nanoscience	Liang-Yan Hsu
TG 4.3	Complex systems	Pik-Yin Lai

Major Academic Personnel:

Center Scientists: TGs are responsible for almost all the academic activities of the Physics Division, and are run by their CSs together with their core members. Currently, there are 32 CSs including 2 honorable CSs (see Table A1.6), who are outstanding scholars from various universities and Academia Sinica, and work in four major fields, namely, TG 1: Quantum Information and Quantum Computing; TG 2: High Energy Physics and Astrophysics, TG 3: Condensed Matter Physics; and TG 4: Interdisciplinary Research. There is no exaggeration to say that the success of the Division depends on the effort of the CSs. It falls on the shoulders of the CSs for leading their TG, mentoring the postdocs as well as students, and promoting the research excellence of the NCTS. On average, each TG has three CSs and one of them is its coordinator.

Table A1.6: List of current 32 Center Scientists (CSs) including 2 honorable CSs.

Name of Center Scientist	TG: Field of research	Period
Hai-Yang Cheng (Honorable CS)	TG2.1: High energy phenomenology	2023.8-present
Ting-Wai Chiu (Honorable CS)	TG2.1: High energy phenomenology	2023.8-present
Hsi-Sheng Goan (NTU)	TG1.1: Quantum computing	2021.1-present
Hao-Chung Cheng (NTU)	TG1.1: Quantum computing	2023.1-present
Chiao-Hsuan Wang (NTU)	TG1.1: Quantum computing	2023.1-present
Wen-Te Liao (NCU) (NTHU)	TG1.2: Quantum physics	2021.1-present
Ray-Kuang Lee (NTHU)	TG1.2: Quantum physics	2021.1-present
Hong-Bin Chen (NCKU)	TG1.3: Quantum information	2023.1-present
Yeong-Cherng Liang (NCKU)	TG1.3: Quantum information	2021.1-present
Shin-Liang Chen (NCHU)	TG1.3: Quantum information	2023.1-present
Cheng-Wei Chiang (NTU)	TG2.1: High energy phenomenology	2021.1-present
Martin Spinrath (NTHU)	TG2.1: High energy phenomenology	2023.1-present
Meng-Ru Wu (IoP-AS)	TG2.1: High energy phenomenology	2023.1-present
Yu-tin Huang (NTU)	TG2.2: High energy theory	2021.1-present
Chong-Sun Chu (NTHU)	TG2.2: High energy theory	2021.1-present
Dimitrios Giataganas (NSYSU)	TG2.2: High energy theory	2023.1-present
Min-Kai Lin (ASIAA-AS)	TG2.3: Astrophysics theory	2021.1-present
Hsi-Yu Schive (NTU)	TG2.3: Astrophysics theory	2021.1-present
Hsiang-Yi Karen Yang (NTHU)	TG2.3: Astrophysics theory	2023.1-present
Feng-Chuan Chuang (NSYSU)	TG3.1: Comp. quantum materials	2021.1-present
Yang-Hao Chan (IoAMS-AS)	TG3.1: Comp. quantum materials	2021.1-present
Tay-Rong Chang (NCKU)	TG3.1: Comp. quantum materials	2022.1-present
Chung-Hou Chung (NYCU)	TG3.2: Strongly correlated systems	2021.1-present
Shin-Ming Huang (NSYSU)	TG3.2: Strongly correlated systems	2023.1-present
Chien-Te Wu (NYCU)	TG3.2: Strongly correlated systems	2021.1-present
Pochung Chen (NTHU)	TG4.1: Computation & machine learning	2021.1-present
Chia-Min Chung (NSYSU)	TG4.1: Computation & machine learning	2023.1-present
Yi-Ping Huang (NTHU)	TG4.1: Computation & machine learning	2023.1-present
Liang-Yan Hsu (IoAMS-AS)	TG4.2: Chemical physics	2023.1-present
Chao-Ping Hsu (IoC-AS)	TG4.2: Chemical physics	2021.1-present
Pik-Yin Lai (NCU)	TG4.3: Complex systems	2023.1-present
Hung-Yan Shih (IoP-AS)	TG4.3: Complex systems	2023.1-present

Postdoctoral Researchers: Well-trained postdoctoral researchers are not only essential for the promotion of the Center's academic excellence but also next generation theoretical scientists. In this new phase of the NCTS, we have introduced two new measures in order to attract young researchers to work in the Center, namely, (1) we review the postdoc positions application every month by the PC, rather than twice a year by the EC in the previous NCTS phase; and (2) we offer competitive salaries which are up to 15 % higher than that set by the NSTC and hosting universities, as well as travel funds for international travels. Thanks to these new measures, we have been able to attract 36 young theorists to work in NCTS in the past two years (see Table A1.7). Currently, the

Division has a research staff consisting of 21 young scientists, namely, 16 postdoctoral researchers (see Table A1.7) and 5 research assistants (see Table A1.8).

Table A1.7: Postdoctoral researchers (36) since 2023 (Currently 16 working in the NCTS).

Name of Researchers	TG: Field of research	Period
Renata Wong (Center)	TG1.1: Quantum computing	2021.11-2023.8
Shih-Kai Chou (Center)	TG1.1: Quantum computing	2024.5-present
Jebarathinam Chellasamy (Center)	TG1.1: Quantum computing	2024.8-present
You-Lin Chuang (NTHU Hub)	TG1.2: Quantum physics	2021.10-2023.9
Shiue-Yuan Shiau (NTHU Hub)	TG1.2: Quantum physics	2018.8-2023;7
Cheng-Wei Huang (NTHU Hub)	TG1.2: Quantum physics	2022.11-2023;1
I-Yun Hsiao (NTHU Hub)	TG1.2: Quantum physics	2024.5-present
Chen-Yu Lee (Center)	TG1.2: Quantum physics	2024.7-present
Shiladitya Mal (NCKU Hub)	TG1.3: Quantum information	2021.8-2023.7
Gelo Noel Tabia (NCKU Hub)	TG1.3: Quantum information	2022.1-2023.12
En-Jui Kuo (NCKU Hub)	TG1.3: Quantum information	2024.1-present
Hugues Beauchesne (Center)	TG2.1: High energy phenomenology	2021.8-2024.7
Yasuhiro Yamamoto (Center)	TG2.1: High energy phenomenology	2021.10-2024.2
Yen-Hsun Lin (Center)	TG2.1: High energy phenomenology	2021.12-2023.7
Mugdha Sarkar (Center)	TG2.1: High energy phenomenology	2022.8-2023.7
Leon Garcia de la Vega (Center)	TG2.1: High energy phenomenology	2023.11-present
Sourav Ballav (Center)	TG2.2: High energy theory	2022.4-2023.9
Himanshu Parihar (NTHU Hub)	TG2.2: High energy theory	2022.11-present
Parthiv Haldar (Center)	TG2.2: High energy theory	2022.12-present
He-Feng Hsieh (Center)	TG2.3: Astrophysics theory	2021.8-2023.7
Hei Yin Jowett Chan (Center)	TG2.3: Astrophysics theory	2022.9-present
Alvina Yee Lian On (NTHU Hub)	TG2.3: Astrophysics theory	2022.12-present
Ashish Kore (Center)	TG3.1: Comp. quantum materials	2022.11-present
Covilakam Sreeparvathy (NSYSU)	TG3.1: Comp. quantum materials	2023.3- present
Aniceto B. Maghirang III (Center)	TG3.1: Comp. quantum materials	2024.9-present
Yung-Yeh Chang (NYCU Hub)	TG3.2: Strongly correlated systems	2021.4-2023.7
Yu-Chin Tzeng (NYCU Hub	TG3.2: Strongly correlated systems	2022.10-2024.7
Kimberly Remund (NYCU Hub)	TG3.2: Strongly correlated systems	2023.9-present
Amrita Ghosh (Center)	TG4.1: Computation & machine learning	2021.9-2023.2
Jozef Genzor (Center)	TG4.1: Computation & machine learning	2021.12-2023.12
Yoshiki Fukusumi (NTHU Hub)	TG4.1: Computation & machine learning	2021.9-2023.2
Fabrizio Giovanni Olivia (NTHU)	TG4.1: Computation & machine learning	2021.9-2023.2
Wei-Chih Chen (Center)	TG4.2: Nanoscale Physics & Chemistry	2021.8-2023.2
Yao-Wen Chang (Center)	TG4.2: Nanoscale Physics & Chemistry	2022.1-present
Chia-Chou Wu (Center)	TG4.3: Complex systems	2022.3-2024.2
Koushik Goswami (Center)	TG4.3: Complex systems	2024.5-present

Nurturing Young Scientists Program:

The cultivation and nurturing of students and young researchers are very important because successful nurturing young talents is our guarantee for a bright future for the science and economy of Taiwan. Therefore, our TGs are requested to provide our young scientists (graduate students and postdocs) with resources (travel money to attend international conferences and schools etc.) and opportunities (to link and bring them to the international platform of research through visiting position, suggestion of speakers etc.) to help them to grow strong. For example, nearly each postdoc is offered a travel grant of about 100,000 NT$ for international conferences or for visiting collaborating overseas research groups. Furthermore, the Division provides training opportunities through organization of schools on advanced level subjects.

Table A1.8: Graduate student research assistants worked in NCTS in 2023 and 2024 (13).

Name	TG:	Site	Period	Current status
Chen, Chi-Chun	TG1.1	NTU	2022.8-2023.5	NTU IBMQ research assistant
Huang, Yu-Chao	TG1.1	NTU	2024.10-present	Working at NCTS
Wu, Chun-Chi	TG1.2	NTU	2022.11-2023.1	U. of Washington, PhD student
Alejandro Q. Trivino	TG1.2	NTHU	2023.4-2023.9	Karlsruhe Inst. of Techn., PhD student
Wang, Hong-Ming	TG1.3	NCKU	2023.3-2023.5	Working in a company
Tsai, Zheng-Lin	TG1.3	NCKU	2024.8-present	Working at NCTS
Wang, Hong-Ming	TG1.3	NCKU	2024.8-present	Working at NCTS
Chen, Yi Xian	TG2.1	NTU	2024.10-present	Working at NCTS
Chen, Chun-Yen	TG2.3	NTU	2024.11-present	Working at NCTS
Wang, Chung-Yu	TG3.1	NTU	2023.11-2024.6	AS Research Assistant
Lin, Jia An	TG3.2	NYCU	2022.11-2023.1	Brown Univ., USA, PhD student
Chang, Heng-Wei	TG3.2	NYCU	2023.4-2023.7	Arizona U., USA, PhD student
Chen, No	TG4.3	NTU	2022.5-2023.1	Syracuse Univ., USA, PhD student

Annual academic awards: To encourage young scholars to engage in theoretical sciences research and to foster outstanding talents in theoretical sciences, the Division has devised three annual awards, namely, (1) Young Theoretical Scholar Award, (2) Postdoc Paper Award and (3) Student Outstanding Paper Award (For more details, see the NCTS webpage: https://phys.ncts.ntu.edu.tw/en/program/young_theorist_award where one can also find the recipients of these awards in the past four years).

Student research fellowship scheme: Many of our graduate students will pursue academic careers after their graduation and will become our future generation of scientists. Usually, there is an interim period before they move onto the next stage in their careers, e.g., applying PhD positions in overseas universities. To encourage these bright students continuing engaged in research and also to give them time writing-up the results of their research carried out while they were a student and also passing-on their expertise to younger members of their former groups, we set up the NCTS student research fellowship scheme in 2021. Thirteen young graduates worked in NCTS in 2023 and 2024 (see Table A1.7). Table A1.7 shows that most of them went on to pursue a PhD degree in either overseas or domestic universities after leaving NCTS. We also notice that many of them completed one or two manuscripts and submitted them for publication during their stay in NCTS.

Interdisciplinary Collaboration and Research Program:
To promote interdisciplinary research and collaboration, as Table A1.8 shows, eleven TGs are grouped into four grand TGs according to their subfields. These four grand TGs are designed to provide platforms for bottom-up collaborations among the regular TGs within it and thus interdisciplinary research. For example, Quantum Information and Quantum Computing (TG 1) are multi-disciplinary fields involving mathematics, physics, chemistry, material and engineering. Thus, the three TGs (TG 1.1, TG 1.2 and TG 1.3) within the grand TG 1 have joint programs such as the joint international conference, joint seminars, workshops and schools. Furthermore, the three TGs are forging long term collaborations with related institutions both in Taiwan and abroad, including the Center of Quantum Technology, Taiwan, IBM Quantum Hub at NTU, Amazon Braket at NCKU, Quantum Computing Research Center at Hon Hai Research Institute, and QFort at NCKU. Furthermore, as the TG 4 title suggests, three TGs in the grand TG 4 are multidisciplinary by nature. In particular, the core members of TG 4.3 consist of not only theoretical physicists but also biologists.

In recent years, machine learning techniques have found their way in sciences, such as identifying phase transitions and topological phases, accelerating simulation algorithms for quantum systems, improving the representation of quantum states, improving signal searches of high energy collision experiments, and pattern analyses of astrophysical data. Fields with big amounts of data such as high energy collision experiments and astronomy are natural candidates to benefit from machine learning which might eventually provide a less theory biased approach to find new theories. Thus, we have supported the collaborations on Machine Learning and Artificial Intelligence across the TGs as well as with Institutions and Companies, such as AI Foundation, Taiwan AI Academy and Brookhaven National Laboratory since 2021.

Experimental Collaboration
Although we have not set up separate experimental collaboration programs, we do provide ample support to our TGs to encourage bottom-up theory-experiment collaborations. For example, in the framework of TG2.1, high energy physics (HEP) experimentalists and phenomenology theorists in Taiwan have formed an integrated group, organizing regular joint mixed online and physical Monday seminars, holding rapid response workshops with both experimental and theoretical participants from USA, Switzerland, China, Japan and Taiwan, helping the experimental groups in Taiwan to make links with the overseas experimental institutions such as the AMS, ATLAS, CMS and Belle II Collaborations.
Furthermore, core members (CMs) of some TGs such as TG 4.3 include experimentalists. By having the theoreticians and experimentalists in the same TG, together they can solve important problems and publish the research outputs in highly prestigious journals such as Nature and Science. In particular, the Nature paper on the emergence of large-scale cell death through ferroptotic trigger waves published in July this year (see Sec. B1 and also TG4.3 report in Sec. II. D), resulted from the collaboration between the experimental core member Sheng-hong Chen and theoretical postdoc Chia-Chou Wu in TG 4.3. Interestingly, some multi-talented CSs such as Ray-Kuang Lee (TG 1.2), have even started doing experiments themselves.

Indeed, our past four years' experience shows that this is in fact a much better way than setting up a separate joint theory-experimental collaboration program.

B. Academic Activities and Major Achievements

B.1 Advancing Research

Table B1.1 NCTS Physics overall research profile and performance in 2023 and 2024.

Indicator	2023	2024[1]
Academic Personnel		
No. of center scientists (CS)	32	32
No. of center postdocs	29	20
No. of graduate student research fellows	4	6
Research Publications		
No. of publications	161	137
No. of publications in high impactful journal[2]	31	33
No. of publications by CSs	96	85
No. of publications by postdocs and research scholars	30	17
Research Activities		
No. of invited plenary talks by CSs	133	87
No. of conferences, workshops, symposium organized	16	13
No. of meetings jointly organized with int'l institutions	9	6
No. of schools organized	7	8
No. of financial support instance to students and postdocs	19	95

Keys: [1] As of 2024/9/30; [2] Journals with top 15 % of impact.

The Division has made significant progress in the advancement on the research in the past two years.

Research publications: The Physics Division published 161 papers in 2023, and has also published 137 papers so far this year. The publications are mostly of high academic quality with highly impactful results appearing in prestigious and competitive journals such as Science and Nature. In particular, thirty-three of them have been published in journals with top 15% of impact in 2024. Please see Table B1.1 for a summary of Division's publications, and also Table B1.2. We notice that compared with other theoretical physics centers and institutions in the world, the research outputs of the Division appear rather outstanding.

Table B1.2 List of the journals in which we published papers in 2023 and 2024.

	Journal (Impact Factor (IF))	2023	2024
1.	ACS Applied Materials & Interfaces (IF: 10.383)	1	
2.	ACS Materials Letters (IF: 9.6)		1

3.	ACS Nano (IF: 18.027)		2
4.	ACS Omega (IF: 4.132)	1	
5.	Advanced Materials (IF: 29.4)	3	
6.	Advanced Quantum Technologies (IF: 4.4)		1
7.	Advanced Science (IF: 15.1)	1	
8.	Annals of Physics (IF: 3)	1	
9.	Applied Physics Letters (IF: 3.971)		1
10.	Astronomy & Astrophysics (IF: 5.4)	1	1
11.	Astrophysical Journal (IF: 4.8)	7	11
12.	Astrophysical Journal Letters (IF: 8.8)		2
13.	Cell Reports Physical Science (IF: 8.9)	1	
14.	Chemical Engineering Journal (IF: 13.3)		1
15.	Chemistry – An Asian Journal (IF: 3.5)		1
16.	Chinese Journal of Physics (IF: 4.6)	2	1
17.	Communications in Mathematical Physics (IF: 2.36)	1	
18.	Communications Physics (IF: 5.4)		2
19.	Computational & Structural Biotechnology Journal (IF: 6)	1	
20.	Computer Physics Communications (IF: 6.2)	1	
21.	Current Opinion in Structural Biology (IF: 6.8)	1	
22.	Dalton Transactions (IF: 4.0)	1	
23.	Energy & Environmental Science (IF: 32.4)		1
24.	Eur. Phys. J. B (IF: 1.6)	1	
25.	Eur. Phys. J. C (IF: 4.2)	3	1
26.	Fortschritte Der Physik – Progress of Physics (IF: 3.9)	1	
27.	Future Generation Computer Systems (IF: 7.5)	1	
28.	Galaxies (IF: 2.5)	3	
29.	Heliyon (IF: 4)	1	
30.	IEEE Journal of Biomedical & Health Informatics (IF: 7.7)	1	
31.	IEEE Nanotechnology Magazine (IF: 2.3)	2	2
32.	IEEE Transactions on Information Theory (IF: 2.2)		2
33.	IEEE Transactions on Emerging Topics in Computational Intelligence (IF: 5.3)	1	
34.	IEEE Transactions on NanoBioscience (IF: 3.7)		1
35.	International Journal of Modern Physics A (IF: 1.4)	1	
36.	Journal of Applied Crystallography (IF: 5.2)		1
37.	Journal of Chemical Physics (IF: 3.1)	2	2

38.	Journal of High Energy Physics (IF: 6.376)	8	10
39.	Journal of Physical Chemistry A (IF: 2.7)	1	1
40.	Journal of Physical Chemistry B (IF: 2.8)		1
41.	Journal of Physical Chemistry C (IF: 3.3)	1	1
42.	Journal of Physical Chemistry Letters (IF: 4.8)	1	1
43.	Journal of Physics A: Mathematical and Theoretical (IF: 2)	1	
44.	Journal of Physics B: Atomic, Molecular and Optical Physics (IF: 1.6)	2	
45.	Journal of Physics G: Nuclear and Particle Physics (IF: 3.4)		1
46.	Journal of the Chinese Chemical Soc. (IF: 1.8)	1	
47.	Machine Learning: Science and Technology (IF: 6.013)		1
48.	Materials Horizons (IF: 12.2)		1
49.	Materials Today (IF: 24.2)	1	
50.	Micromachines (IF: 3.4)	1	
51.	Molecules (IF: 4.2)	1	2
52.	Monthly Notices of the Royal Astronomical Society (IF: 4.7)	7	4
53.	Nano Energy (IF: 16.8)		2
54.	Nano Letters (IF: 9.6)	3	1
55.	Nanomaterials (IF: 5.719)	2	1
56.	Nanoscale Advances (IF: 5.598)	1	
57.	Nanoscale Horizons (IF: 9.7)	1	
58.	Nature (IF: 50.5)		1
59.	Nature Astronomy (IF: 14.1)	1	
60.	Nature Communications (IF: 14.7)	5	5
61.	Nature Electronics (IF: 33.7)		1
62.	Nature Materials (IF: 47.656)	1	
63.	Nature Physics (IF: 19.684)		2
64.	New Journal of Physics (New J. Phys.) (IF: 3.716)	3	4
65.	npj 2D Materials and Applications (IF: 10.516)		1
66.	npj Quantum Information (IF: 10.758)		1
67.	npj Quantum Materials (IF: 6.856)	1	1
68.	Optics & Laser Technology (IF: 4.6)		1
69.	Optics Communications (IF: 2.2)		1
70.	Optics Express (Opt. Express) (IF: 3.833)	2	

71.	Optics Letters (IF: 3.6)	1	
72.	Physica B: Condensed Matter (IF: 2.6)		3
73.	Physica Scripta (IF: 2.8)		
74.	Physical Review A (IF: 2.6)	6	5
75.	Physical Review B (IF: 3.2)	20	10
76.	Physical Review C (IF: 3.2)		1
77.	Physical Review D (IF: 4.6)	10	15
78.	Physical Review E (IF: 2.2)	5	2
79.	Physical Review Letters (IF: 8.1)	5	3
80.	Physical Review Materials (IF: 3.4)	3	
81.	Physical Review Research (IF: 3.5)	11	7
82.	Physical Review X (IF: 11.6)		1
83.	Physics Letters B (IF: 4.3)	2	1
84.	PNAS (IF: 12.779)	2	
85.	Progress in Particle and Nuclear Physics (IF: 14.5)		1
86.	PRX Quantum (IF: 7.514)	1	
87.	Quantum (IF: 5.1)	4	2
88.	Quantum Information Processing (IF: 2.2)		1
89.	Quantum Science and Technology (IF: 5.6)		2
90.	Quantum Studies – Mathematics and Foundations (IF: 0.8)	1	
91.	RSC Adv. (IF: 3.9)	1	
92.	Science (IF: 44.7)	1	1
93.	Scientific Reports (IF: 4.997)	2	
94.	SciPost Physics (IF: 4.6)		1
95.	Surface Science (IF: 2.1)		1
96.	Universe (IF: 2.5)		1
Sum		161	137

Highlights of publications: Here we present a few selected papers published in 2023 and 2024 by the members of the NCTS Physics. You can also find other significant papers published in the past two years in the reports from the reports of Thematic Groups in Sec. II and articles from Center Scientists in Sec. III. A in this Biannual Report.

Year 2023

(1) **Is the Decay of the Higgs Boson to a Photon and a Dark Photon Currently**

Observable at the LHC?

[Hugues Beauchesne (postdoc) and Cheng-Wei Chiang (TG 2.1), Phys. Rev. Lett. 130, 141801 (2023)]

The potential decay of the Higgs boson to a photon and a massless dark photon has been the subject of multiple dedicated searches at the LHC. For this decay to be realistically observable, new mediators that communicate between the standard model particles and the dark photon must exist. In this work, we studied constraints on these mediators coming from the Higgs signal strengths, oblique parameters, electric dipole moment of the electron, and unitarity (Fig. B1.1). We found that this branching ratio is far more constrained than previously expected, putting into question the possibility of ever observing this decay at the LHC.

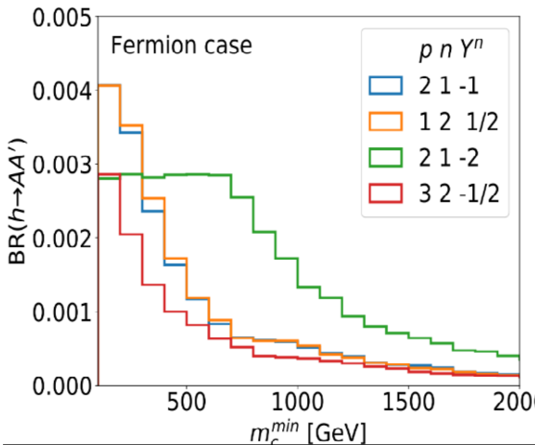


Fig. B1.1 Maximum allowed BR ($h \to AA'$) for Fermion case of mediator models. The plots do not go below 100 GeV, as LEP bounds would prohibit charged particles of such masses.

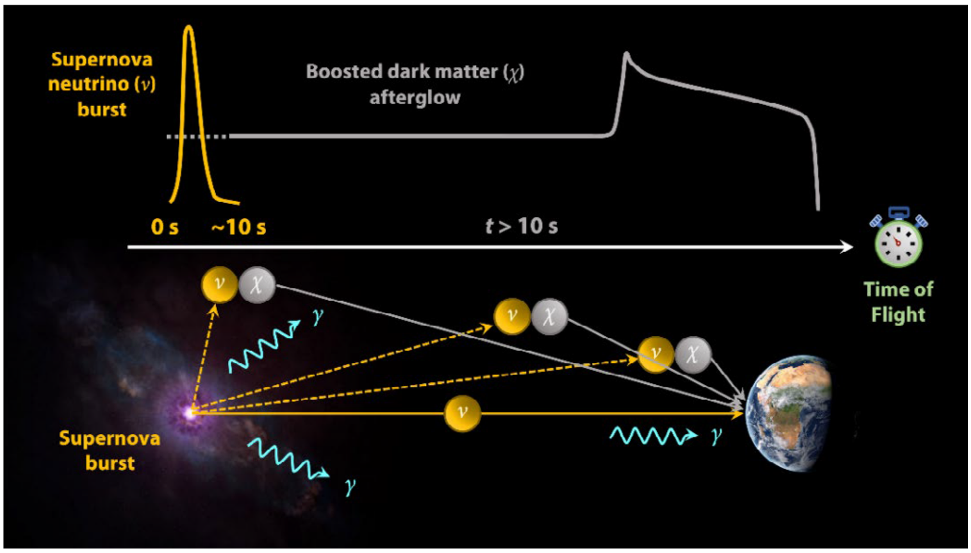


Fig. B1.2 Schematics of neutrino afterglows due to supernova explosions.

(2) **New Experimental signatures added to the arsenal for dark matter searches**

[Yen-Hsun Lin (postdoc), Meng-Ru Wu (TG 2.1) + coworkers, Phys. Rev. Lett. 130, 111002 (2023)]

We identified a novel concept of using "afterglows" of supernova explosions due to Dark Matter (DM) interactions in detectors as new experimental signatures to Direct DM searches. The conventional approach of DM detection via its elastic scattering with the nucleus is restricted by small observable energies and the lack of complementary information. Supernova neutrinos (SNν) can transfer their kinetic energy to the DM in the cosmos. Upon arrival on Earth, these boosted-DM (BDM) would produce distinctive observables in large detectors. In addition, the

Time-of-Flight distribution of the BDM events relative to the initial SNs neutrino burst are smoking-gun signatures for DM. A positive detection of SNνBDM can provide powerful constraints to DM masses and interaction cross-sections. Limits derived by this analysis on SN1987a with data from the Super-Kamiokande experiment exceed the current bounds from BDM due to cosmic-rays by several orders of magnitude. The sensitivity reaches of future detections of BDM due to SNν from the Galactic Center is projected, indicating potentials to probe a vast parameter space not previously accessible in DM searches.

(3) **Einstein rings modulated by wavelike dark matter from anomalies in gravitationally lensed images**

[His-Yu Schive (TG 2.3) +coworkers, Nature Astronomy 7, 736 (2023)]

Leading candidates for dark matter (DM) are weakly interacting massive particles or ultralight bosons (axions), at opposite extremes in mass scales. Whereas DM weakly interacting massive particles behave like discrete particles (ϱDM), quantum interference between DM axions is manifested as waves (ψDM). An international team, comprising Prof. Hsi-Yu Schive (TG2.3 CS) and Prof. Tzihong Chiueh (NTU), shows that gravitational lensing leaves signatures in multiply lensed images of background galaxies that reveal whether the foreground lensing galaxy inhabits a ϱDM or ψDM halo. ψDM lens models correctly predict the level of anomalies remaining with ϱDM lens models. Moreover, when subjected to a battery of tests for reproducing the quadruply lensed triplet images in the system HS 0810+2554, ψDM is able to reproduce all aspects of this system. The ability of ψDM to resolve lensing anomalies tilt the balance toward new physics invoking axions.

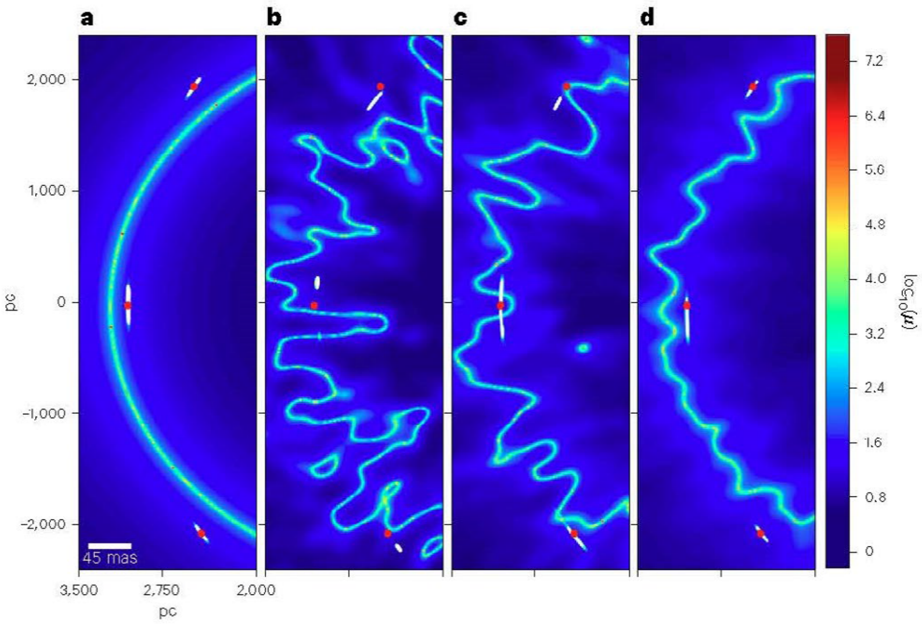


Fig. B1.3 Lensing magnification of ρDM(a) vs ΨDM (b-d) halos.

(4) **Axion optical induction of antiferromagnetic order**

[Tay-Rong Chang and Hsin Lin (TG 3.1) + coworkers, Nature Mater. 22 (2023) 583]

Using circularly polarized light to control quantum matter is a highly intriguing topic in physics, chemistry and biology. Previous works have demonstrated helicity-dependent optical control of chirality and ferromagnetic states. In this work, we discover that the circularly polarized light can control the antiferromagnetic (AFM) order in a 2D even-layer axion insulator $MnBi_2Te_4$ (Fig. B1.4). Our work shows that the optical control and circular dichroism both arise from the optical axion electrodynamics.

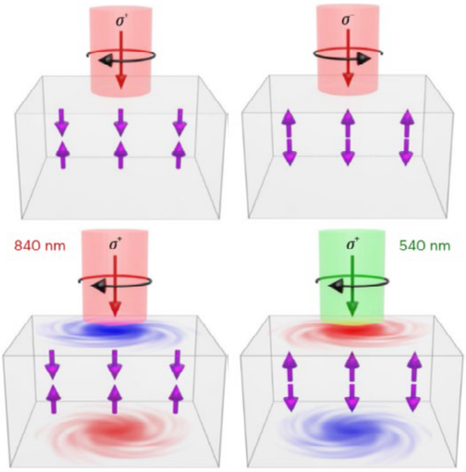


Fig. B1.4 Schematic illustration that circularly polarized induction light ($\lambda_{induction}$ = 840 nm and 540 nm) is shined on sample ($MnBi_2Te_4$ flake on a sapphire substrate) (upper panels), which induce the Berry curvature real-space dipole (bottom panels).

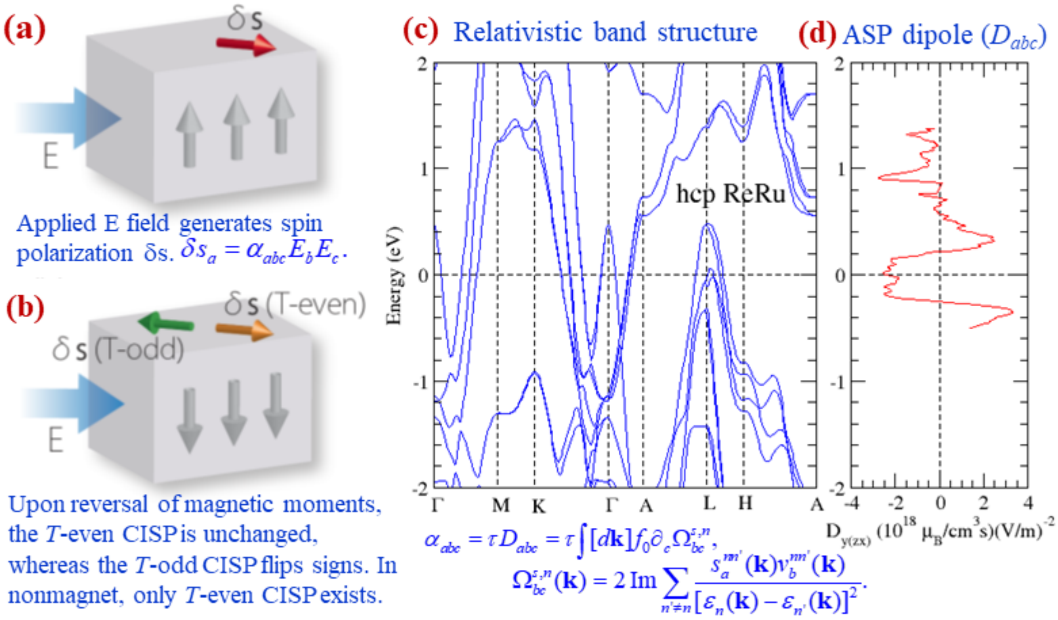


Fig. B1.5 (a-b) Schematic figure showing the difference between *T*-even and *T*-odd current induced spin polarization (CISP). (c) Relativistic band structure and (d) anomalous spin polarization (ASP) dipole (D_{abc}) of hcp ReRu.

(5) **Time-reversal-even nonlinear current induced spin polarization in centrosymmetric solids**

[Guang-Yu Guo (TG 3.1) + coworkers, Phys. Rev. Lett. 130 (2023) 166302]

The quantum spin Hall (QSH) phase is a topological quantum phase that features a 2D insulating bulk and a helical edge state. Here we use vector magnetic field and variable temperature based STM to provide micro-spectroscopic evidence for a room-temperature QSH edge state on the surface of the higher-order topological insulator Bi_4Br_4. We find that the atomically resolved lattice exhibits a large insulating gap of over 200 meV, and an atomically sharp monolayer step edge hosts an in-gap gapless state. An external magnetic field can gap the edge state, consistent with the time-reversal symmetry protection inherent in the underlying band topology. We further identify the geometrical hybridization of such edge states, which not only supports the Z_2 topology of the quantum spin Hall state but also visualizes the building blocks of the higher-order topological insulator phase. Our results further encourage the exploration of high-temperature transport quantization of the putative topological phase reported here.

(6) **Statistical laws of stick-slip friction at mesoscale**

[Pik-Yin Lai and Hsuan-Yi Chen (TG 4.3) + coworkers, Nature Commun. 14 (2023) 6221]

Friction between two rough solid surfaces often involves local stick-slip events occurring at different locations of the contact interface. If the apparent contact area is large, multiple local slips may take place simultaneously and the total frictional force is a sum of the pinning forces imposed by many asperities on the interface. Here, we report a systematic study of stick-slip friction over a mesoscale contact area using a hanging-beam lateral atomic-force-microscope, which is capable of resolving frictional force fluctuations generated by individual slip events and measuring their statistical properties at the singleslip resolution. The measured probability density functions (PDFs) of the slip length δx_s, the maximal force F_c needed to trigger the local slips, and the local force gradient k' of the asperity-induced pinning force field provide a comprehensive statistical description of stick-slip friction that is often associated with the avalanche dynamics at a critical state. In particular, the measured PDF of δx_s obeys a power law distribution and the power-law exponent is explained by a new theoretical model for the under-damped spring-block motion under a Brownian-correlated pinning force field. This model provides a long-sought physical mechanism for the avalanche dynamics in stick-slip friction at mesoscale.

Year 2024

(7) **New Diffuse boosted dark matter background from all galaxies in the Universe**

[Yen-Hsun Lin (postdoc), Meng-Ru Wu (TG 2.1) + coworkers, Phys. Rev. Lett. 133, 111004 (2024)]

We have considered a novel component of the diffuse boosted dark matter (DBDM) driven by all past supernova explosions that happened in the Universe. This DBDM, akin to the renowned diffuse supernova neutrino background, offers a new perspective in dark matter detection. Our analysis reveals that

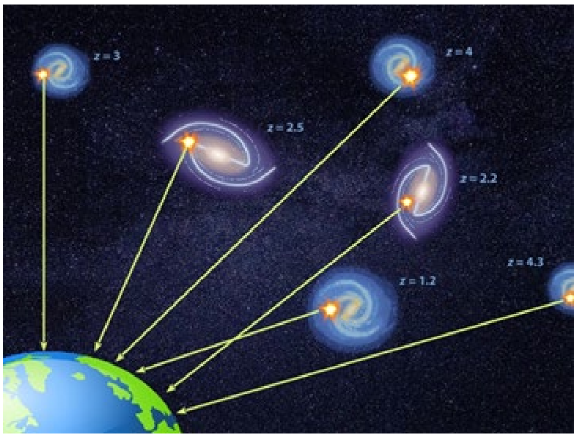


Fig. B1.6 Schematic picture showing the diffuse boosted dark matter from supernova explosions in all galaxies in the Universe.

DBDM not only can provide improved sensitivities to probe the unknown nature of DM with just a few years of exposure time from the upcoming neutrino experiment Hyper-Kamiokande compared to earlier studies, but also proves robust against uncertainties originated from the dark matter profiles in different galaxies. This work highlights a new way to utilize our understanding of astrophysical transients to probe the fundamental particle physics (Fig. B1.6).

(8) **Observation of possible excitonic charge density waves and metal-insulator transitions in atomically thin semimetals**
[Yang-Hao Chan (TG 3.1) + coworkers, Nature Phys. 20 (2024) 597] (Fig. B1.7)
In solids, the condensation of electron and hole pairs with finite momentum leads to an ordered state known as a charge density wave. The origin of the transition has been debated as lattice symmetry breaking and the accompanying relocation of the ions can also lead to changes the charge distribution. Here we demonstrate a condensed phase in low-dimensional $HfTe_2$. Angle-resolved photoemission spectroscopy measurements reveal a metal–insulator transition and the emergence of replica bands at low temperature which are consistent with a charge density wave ground state. Raman spectroscopy shows no sign of lattice distortion within the detection limit. Our results indicate a possible excitonic insulator phase in low-dimensional $HfTe_2$ without any structural modification.

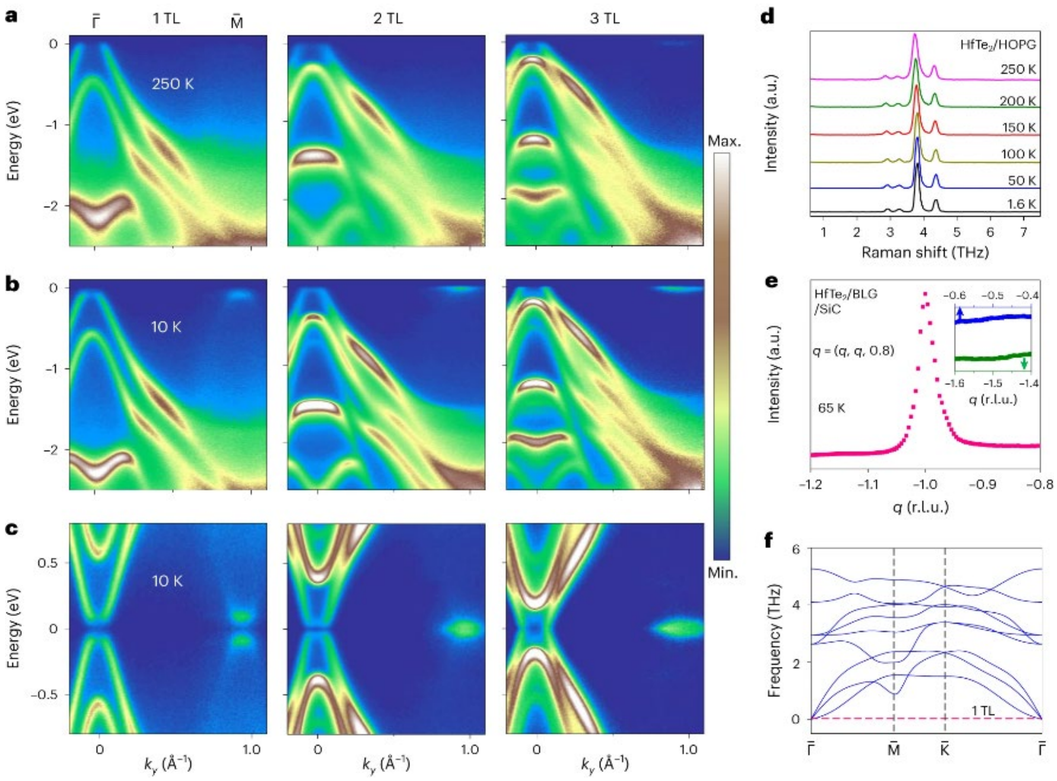


Fig. B1.7 Thickness dependence of the band structure and phonon dispersions of 2-D $HfTe_2$.

(9) **Proximity induced charge density wave in a graphene/1T-TaS2 heterostructure**
[Horng-Tay Jeng (TG3.1) + Chung-Hou Chung (TG3.2) + coworkers, Nature Commun. 15, 8056 (2024)]
Proximity-effect is widely used to induce correlated states, such as superconductivity or magnetism, at heterostructure interfaces.

However, demonstrating the existence of proximity-induced charge-density waves (PI-CDW) has been challenging. This is due to competing effects, such as screening or co-tunneling into the parent material, that obscured its presence. Here we report the observation of a PI-CDW in a graphene layer contacted by a 1T-TaS_2 substrate. Using STM and STS spectroscopy together with theoretical-modeling, we show that the coexistence of a CDW with a Mott–gap in 1T-TaS_2 coupled with the Dirac-dispersion of electrons in graphene, makes it possible to unambiguously demonstrate the PI-CDW. We further show that the mechanism underlying the PI-CDW is the short-range exchange-interactions that are distinctly different from previously observed proximity effects.

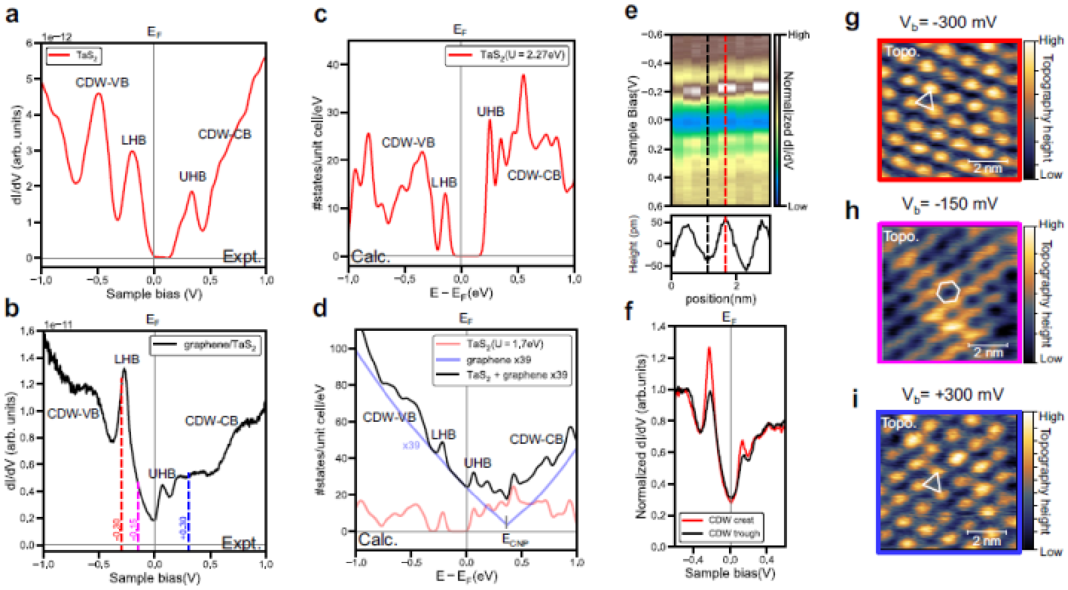


Fig. B1.8 Effects of interaction between graphene and 1T-TaS_2. **a**, **b** are the measured dI/dV curves. **c**, **d** are the calculated DOS for bulk 1T-TaS_2 and the heterostructure, respectively. **e** A map of dI/dV vs position across 8 DSs in graphene/1T-TaS2. **g-i**.STM topography scans measured at voltages of -300 mV, -150 mV and +300 mV, respectively.

(10) **Coexistence of superconductivity with partially filled stripes in the Hubbard model**

[Chia-Min Chung (TG 4.1 CS) + coworkers, Science 384, eadh7691 (2024)] (Fig. B1.9)

Combining the complementary capabilities of two of the most powerful modern computational methods, the authors found superconductivity in both the electron- and hole-doped regimes of the two-dimensional Hubbard model. In the electron-doped regime, superconductivity is weaker and is accompanied by antiferromagnetic Neel correlations at low doping. The strong superconductivity on the hole-doped side coexists with stripe order, which persists into the overdoped region with weaker hole density modulation. These stripe orders, neither filled as in the pure Hubbard model nor half-filled as seen in previous state-of-the-art calculations, vary in fillings between 0.6 and 0.8. These results validate the applicability of this iconic model for describing cuprate high-T_c superconductivity.

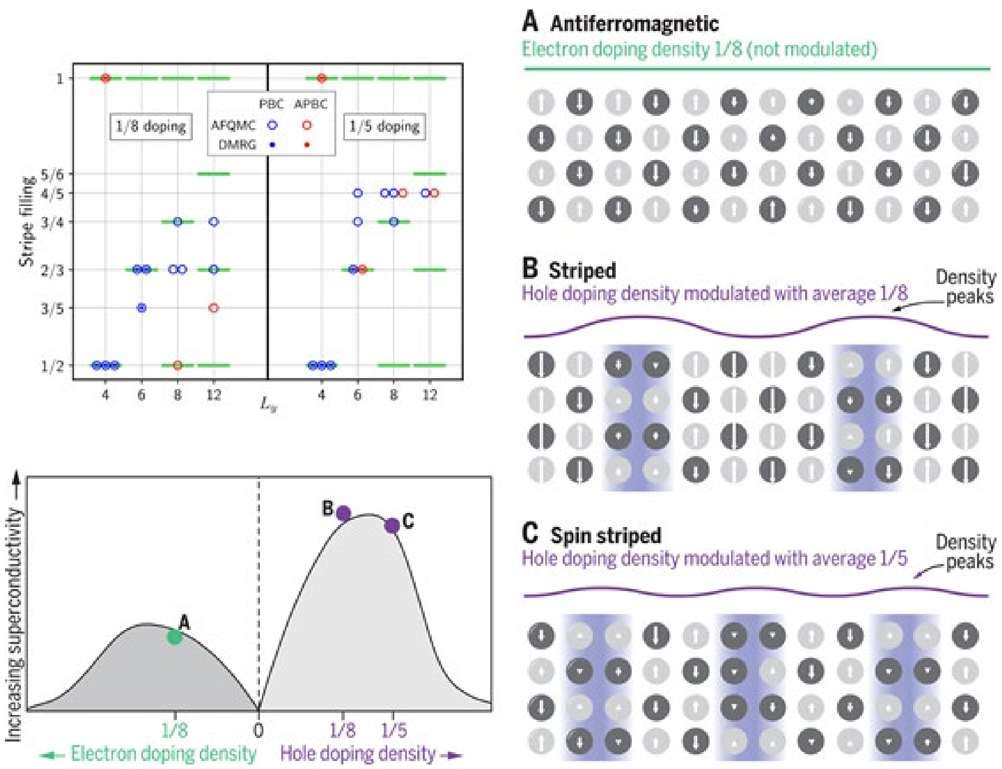


Fig. B1.9 (upper left) Partially filled stripe patterns on the hole-doped side at δ = 1/8 and 1/5. (lower left) Phase diagram of the computed pairing-order parameter. (A-C) Spin structure, charge striped and spin-charge striped structure in the hole-doped *t-t'-U* Hubbard model.

(11) **Emergence of large-scale cell death through ferroptotic trigger waves**

[TG 4.3: Sheng-hong Chen (CM), Chia-Chou Wu (Postdoc) + coworkers, Nature 631, 654 (2024)]

Large-scale cell death is commonly observed during organismal development and in human pathologies. These cell death events extend over great distances to eliminate large populations of cells, raising the question of how cell death can be coordinated in space and time. In this paper, the authors show that ferroptosis, an iron- and lipid-peroxidation-dependent cell death, propagates across human cells over long distances (≥ 5 mm) at constant speeds (~5.5 μm min^{-1}) via reactive oxygen species (ROS) trigger waves. ROS feedback loops control wave progression. Ferroptotic stress activates these loops, creating bistable cellular redox systems that enable ROS propagation. They demonstrate ferroptosis's role in embryonic avian limb muscle remodeling, suggesting its function in tissue sculpting during embryogenesis. These findings reveal ferroptosis's importance in coordinating large-scale cell death, offering insights into embryonic development and human pathologies. It should be noted that this superb paper has resulted from the fruitful collaboration between an experimental CM and a theoretical postdoc in the same TG.

(12) **Avalanches and Extreme Value Statistics of a Mesoscale Moving Contact Line**

[Hsuan-Yi Chen, Pik-Yin (TG 4.3) + coworkers, Phys. Rev. Lett. 132, 084003 (2024)] (Fig. B1.10)

The pinning-depinning dynamics of a circular moving contact line (CL) over the rough surface of a micron-sized vertical hanging AFM glass fiber are analyzed. The capillary force acting on the CL exhibits sawtooth-like fluctuations, with a linear accumulation of force of slope k (stick) followed by a sharp release of force δf, which is proportional to the CL slip length. We find that the local maximal force Fc needed for CL depinning follows the extreme value statistics and the measured δf follows the avalanche dynamics with a power law distribution in good agreement with the Alessandro-Beatrice-Bertotti-Montorsi model. The results provide an accurate statistical description of the CL dynamics at mesoscale, which has important implications to a common class of problems involving stick-slip motion in a random defect or roughness landscape.

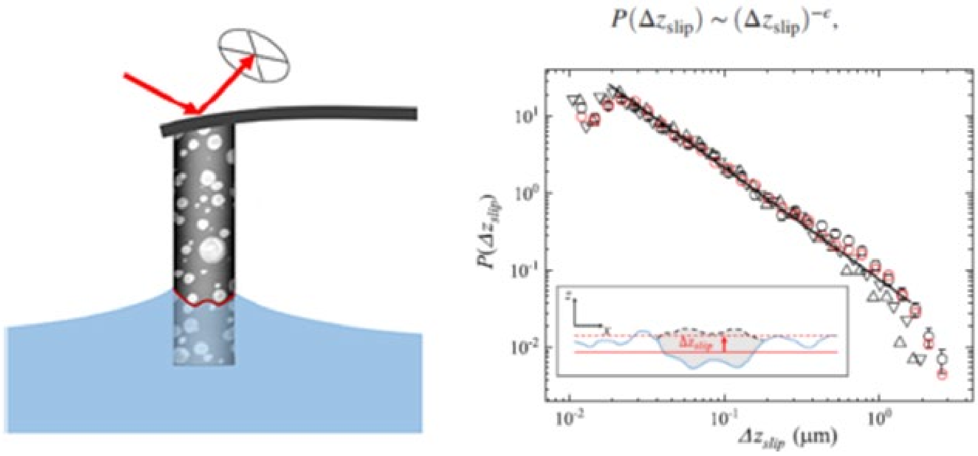


Fig. B1.10 Left: Schematic of the long-needle AFM probe of a glass fiber, forming a liquid-air interface and a circular contact line. Right: The slip length for different scanning speeds obeys a power law as predicted.

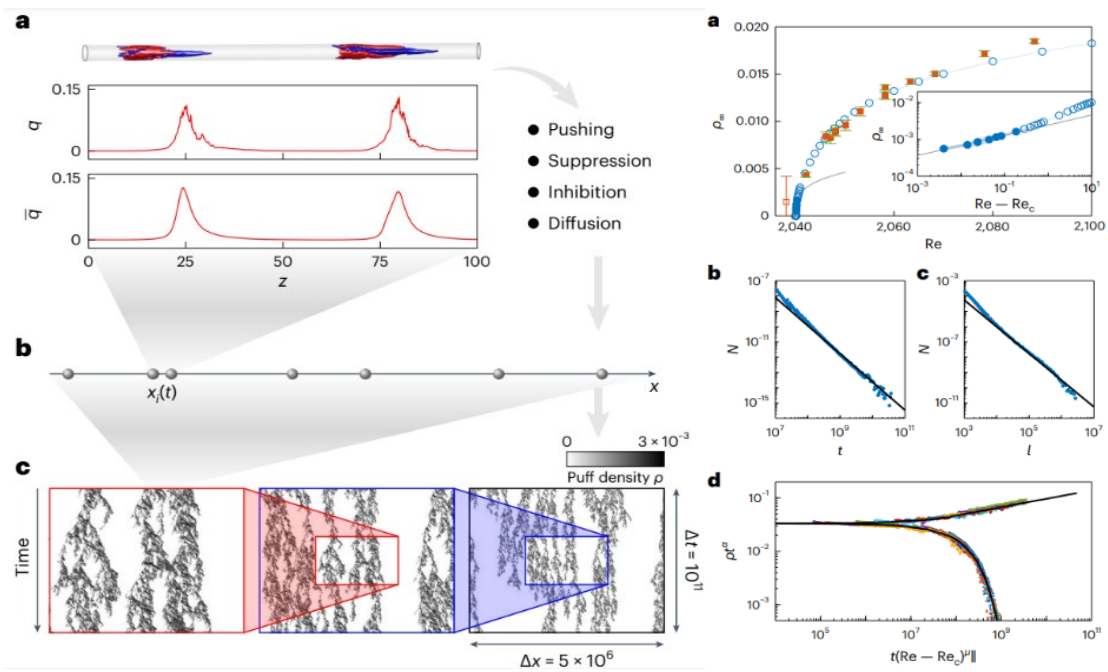


Fig. B1.11 Illustration of the bottom-up multiscale approach to the laminar–turbulent transition in pipe flow used in this study. **a**, Instantaneous turbulent kinetic energy of the perturbation averaged over the cross-section of the pipe from a DNS showing two interacting turbulent puffs. **b**, A mesoscale model describes puffs as point particles interacting in a one-dimensional domain and is solved numerically. **c**, At the macroscopic scale, statistical mechanics analytically and numerically yields the phase diagram and detailed transitional behavior of the flow.

(13) **Directed percolation and puff jamming near the transition to pipe turbulence**

[Hong-Yan Shih (TG 4.3 CS) + coworkers, Nature Physics 20, 1339 (2024)] (Fig. B1.11)

Recent theoretical and experimental studies have advanced progress in understanding the transitional turbulence and suggest that it is a directed percolation non-equilibrium phase transition, but whether it is generic in pipe flow is still unclear due to the limitation of the extremely long-time scales near transition. Combining experimental measurements and numerical simulations and renormalization group analysis of minimal models, we find a jammed phase of puffs with pairwise interactions emerging above the critical point and confirm that the turbulent fraction follows the critical scaling of directed percolation. Our work shows that statistical mechanics can provide quantitative understanding and predictions to turbulent flows.

B.2 Center Scientist and Thematic Group Programs

Research publications. The performance of the CS Program is rather impressive and has led to the publication of about 96 and 85 papers, respectively, in 2023 and 2024 (see Table B1.1), which are about 60 % and 62 % of the academic papers of the Division, respectively. Here, let me provide a few examples. In particular, the achievements of some CS and core members are truly outstanding. In 2023, Tay-Rong Chang, Feng-Chuan Chuang and Yang-Hao Chan (TG 3.1 CS) have published 12, 6 and 5 papers, respectively, in the name of NCTS and most of these papers are in the prestigious journals such as Science, Nature Materials, PNAS and Nano Letters (see TG 3.1 Report in Appendix II). Hao-Chung Cheng (TG 1.1 CS) and his coworkers have published 7 papers in the name of NCTS. Meng-Ru Wu has also published 8 papers this year and most of them are in the important physics and high energy physics journals, e.g., Phys. Rev. Lett. and Phys. Rev. D and JHEP (see TG 2.1 Report in Appendix II). Very impressively, Tay-Rong Chang (TG 3.1 CS) and His-Yu Schive (TG 2.3 CS) have published a paper in the highly competitive journal Nature Materials and Nature Astronomy, respectively (see Highlights of publications in Sec. B.1 above). Importantly, collaboration has been rather strong as can be seen from the many collaborative publications of the CS research teams.

Research teams. Individual TGs are successfully building up their research teams with postdocs and research students. Together, each team as a whole interacts with other domestic or international collaborators, and students in the community, to engage in active research on frontier research topics (see Sec. I. A.2, Sec. II and Sec. III).

Recognition. The academic achievements of the NCTS Physics members have been recognized by various national and international honors and awards in the past two years, as listed in Table 3.3 in Sec. 3.3, Reports of Thematic Groups in Appendix III as well as the announcements on the NCTS Physics website https://phys.ncts.ntu.edu.tw/ . Among the young NCTS Physics members, in particular, Min-Kai Lin (TG 2.3 CS) won the 10th FAOS Young Scholars' Creativity Award. Karen Hsiang-Yi Yang (TG 2.3 CS) received the prestigious NSTC Ta-You Wu Memorial Award in 2023. Among the senior NCTS Physics members, for example, Ray-Kuang Lee (TG 1.2 CS) became an elected Optica (formerly Optical Society of America) Fellow in 2023. Domestically, Horng-Tay Jeng (TG 3.1 CM), Chao-Ping Hsu (TG 4.2 CS) and Ray-Kuang Lee were awarded the competitive

NSTC Outstanding Research Award this year. Finally, Pei-Ming Ho (TG 2.2 CM) won the MOE 67th Academic Award, and Guang-Yu Guo (TG 3.1 CM) won the MOE 27th National Chair Professor in 2023.

For further information, please see the reports of Thematic Groups and CSs in Sec. II and Sec. III, respectively.

B.3 Nurturing Young Scientists

Nurturing of young scientists, giving them support and helping them to fully develop their potential so as to make significant contributions in the frontier of research subjects is an important mission of the NCTS. In Phase V, this task of nurturing has been performed through a number of projects. Firstly, Physics Division organizes our advanced schools and workshops each year. Secondly, Physics Division supported international exchange program and visitor program. Thirdly, we have also devised three annual NCTS Awards series, the Young Theorist Award, Postdoc Best Paper Award and Student Outstanding Paper Award (see the NCTS webpage link: https://phys.ncts.ntu.edu.tw/en/program/young_theorist_award for the regulations of these awards) in order to encourage young scholars to engage in theoretical sciences research and to foster outstanding talents in theoretical sciences. The webpage link also lists the winners of the Young Theorist Award, Postdoc Best Paper Award and Student Outstanding Paper Award since 2021. In fact, to promote the achievements of our NCTS Young Theorist Awardees, we organize the Young Theorist Award Ceremony in the TPS annual conference each year and also invite them to deliver an invited talk in the Theoretical Physics Symposium in the TPS conference.

Fig. B3.1 Photo taken in the 2023 NCTS Student Outstanding Paper Award Ceremony and Workshop.

The Student Outstanding Paper Award scheme was established in 2021. My participation of the selection processes in the past years make me feel that many of our students are much brighter and much more capable than we thought. I was really impressed by the high quality of the papers submitted in their applications. In particular, eight applications were successful in 2023 and nice surprisingly, three of the selected papers were published in Phys. Rev. Lett., one in Nature Communs. and one in Science Advances. It is definitely worthwhile to invest on our young scholars.

As mentioned before, in 2021 we also launched the *student research fellowship scheme* to encourage the bright graduate students continuing their research and also to give them time writing-up the results of their research carried out while they were a student and also passing-on their expertise to younger members of their former groups, before moving onto the next stage of their academic careers. Thirteen young graduates have been hired in 2023 and 2024 (see Table A1.7). Many of them completed one or two manuscripts and submitted them for publication during their stay in the NCTS. Table A1.7 shows that after leaving the NCTS, majority of them went onto pursue a PhD degree in either overseas or domestic universities.

Some innovative measures to cultivate young students were also introduced by some TGs.
Summer Student Program: TG 2.3 Theoretical and Computational Astrophysics (TCA) group organizes a two-month long Summer Student Program (SSP) annually to provide aspiring junior astronomers with hands-on research experience since 2021. As a further incentive, the NCTS Physics offers each student a studentship of 20,000 NTD / month. The SSP has approximately 15 students annually and includes international students, though the latter participates remotely. Unlike other centrally organized summer programs, the TCA SSP is unique in its approach: faculty and postdocs from across Taiwan can take on students who are dispersed to those institutions for their research projects. This is a precious resource for institutions or departments lacking a summer program, as it allows them to take on summer students through NCTS.

Young Researcher and Student Forum: To train students and young researchers, TG 1.1 initiated a young researcher and student forum which is organized by themselves in 2023. They meet weekly in the NCTS Physics Lecture Hall during semester and the meetings start at noon with lunch boxes provided by the NCTS. Through different kinds of talks, journal club and/or study groups where students and young researchers could develop essential skills of literature search, scientific communications, and oral presentations, enhancing their professional development. Moreover, brining young researchers and students from different groups together could promote research creativity and facilitate collaborations.

Highlights of achievements:
(1) *Schools, hands-on courses and workshops:* In 2023, we organized 8 advanced schools and hands-on courses, aiming at students as well as young postdocs, as listed in Table B3.1. Each of them attracted about 100 or more young researchers, and thus totally several hundreds of students and postdoctoral researchers have been benefited. We have organized more advanced schools and hands-on courses this year. Seven prominent schools are listed in Table B3.2. Most of them attracted tens of participants each, and some of them attracted over 100 young researchers (see Table B3.2).

Table B3.1: An incomplete list of NCTS schools organized in 2023

NCTS Schools	Participants	Date
2023 NCTS summer school on non-Hermitian and non-equilibrium quantum many-body systems	75	2023/8/31-9/1
2023 Summer school on First Principles Computational Materials Research- Advance Level	58	2023/8/28-9/1
2023 Tensor Network and Quantum Computing for Strongly Correlated Systems	25	2023/8/28-8/30
2023 AMO Summer School	60	2023/8/22-8/25
NCTS-TCA Summer Student Program 2023	75	2023/7/01-8/31
2023 Summer school on First Principles Computational Materials Research- Introductory Level	148	2023/6/26-6/27
The 2nd NCTS/UCAT/NTHU International Astronomy Winter School	171	2023/1/31-2/4
NCTS 2023 Frontiers of Complex Systems Winter School	82	2023/1/15

Table B3.2: An incomplete list of NCTS schools organized in 2024

NCTS Schools	Participants	Date
NCTS 2024 Frontiers of Complex Systems Winter School	64	2024/1/23
2024 Summer school on First Principles Computational Materials Research- Introductory Level	160	2024/6/24-6/25
Joint NCTS Phys-Math Summer School on Quantum Information	92	2024/6/25-6/27
NCTS-TCA Summer Student Program 2024	121	2024/7/1-7/3
2024 Mini-workshop: Advanced Tensor Network Applications	11	2024/7/31-8/1
2024 Strongly Correlated Physics, Numerical and Analytical Approaches	72	2024/8/5-8/8
2024 Atomic, Molecular and Optical Physics Summer School	80	2024/8/12-8/15
2024 Summer School on First Principles Computational Materials Research - Advance Level	74	2024/08/12-8/16

(2) *Enhancing experience and visibility:* We allocate a considerable amount of travel fund each year to support the overseas visits of our students and postdocs in order to help them to promote their research and to increase their visibility in the international community, thus helping them to secure a further job position. In particular, we encourage students and postdocs to actively participate and give presentations in international conferences hosted by both NCTS TGs and overseas organizations. As Table B3.3 indicates, we support 15 and 11 students and research assistants, respectively, in 2023 and 2024 to attend international conferences and also to carry out collaborative research overseas. Similarly, we also support 18 and 9 postdocs to participate international activities overseas in 2023 and 2024, respectively.

Table B3.3: Instances of our students and postdocs participating international activities

	International Activity	2023	2024 (as of 10/31)
Students:	Research visits	2	0
(including RAs)	Talks/attendance at int'l conferences	13	11
	sub-total	15	11
Postdocs:	Research visits	6	2
	Talks/attendance at int'l conferences	12	7
	sub-total	18	9
Total:		33	20

B.4 Enhancing International Cooperation and Collaboration

Multilateral joint workshops and conferences: In the past two years, we have continued making our strenuous efforts to promote international cooperation through organizing international conferences and workshops, and also supporting the international visitor programs. For example, Tables B4.1 and B4.2 show that the Division has already had four either bilateral or multilateral workshops so far, and three more are planned and will be held in October and November this year.

Table B4.1: Joint international meetings organized by NCTS in 2023

Joint Meetings	Participants	Involved parties	Date
2023 NCTS Annual Theory Meeting: Particle Physics, String Theory, Cosmology, and Astrophysics	75	Japan, Korea, UK, USA, Taiwan	2023/12/15-12/17
NCTS-ASIAA Large-scale Parity Violation Workshop	84	Amsterdam, Canada, Hong Kong, India, Japan, Korea, Spain, Taiwan, UK, USA	2023/12/04-12/7
14th Taiwan String Workshop	63	France, Japan, Korea, Taiwan, UK	2023/10/30-11/5
27th International Summer Institute on Phenomenology of Elementary Particle Physics and Cosmology	79	Australia, Germany, Japan, Korea, Morocco, USA	2023/8/21-8/25
STATPHYS28 Satellite Meeting – Emergence in Biological Networks	104	China, Germany, Hong Kong, Japan, Taiwan, UK, USA	2023/7/31-8/2
The First International Advisory Committee (IAC) Meeting	42	France, Israel, Japan, Korea, Taiwan, USA	2023/06/20-6/21
The Future is non-perturbative	56	Japan, Poland, Switzerland, Taiwan, USA	2023/6/07-6/09
2023 NCTS-KIAS Workshop on Ab Initio Approaches to Quantum Materials	80	Korea, Taiwan	2023/4/27-4/29
Taiwanese-German Young Researchers Forum on Quantum Information Science	85	Germany, Sweden, Taiwan	2023/2/17-2/19

Table B4.2: Joint international meetings organized by NCTS in 2024

Joint Meetings	Participants	Involved parties	Date
JUST: Japan-US-Taiwan Particle Physics Workshop	51	US, Japan, Taiwan	2024/06/10-06/13
International Workshop on Transport and Optics in	60	Japan, Taiwan, USA, Germany	2024/06/12-06/14
10th Galaxy Evolution Workshop	121	Japan, Korea, Taiwan	2024/08/06-
NCTS-iTHEMS (RIKEN) Joint Workshop on Mater to Spacetime: Symmetries and Geometry	51		2024/08/25-08/29
The Fifteenth Particle Physics Phenomenology Workshop	TB held	Taiwan, Japan, Korea, HK, Germany, Italy, USA, Spain	2024/10/21-10/24
2024 Workshop on Applications of Machine Learning and Artificial Intelligence for Physics and	TB held	Taiwan, China, Japan, Korea	2024/11/08-11/09
2024 East Asia Joint Workshop on Fields and Strings (EAJW)	TB held	Taiwan, Japan, Korea	2024/11/18-11/22

International networks: Since its establishment, NCTS Physics has developed bilateral agreements with 14 international institutions and centers in order to foster scientific collaboration (Fig. B4.1). In particular, in December, 2022, the NCTS signed a 5-year MOU with RIKEN-iTHEMS (Interdisciplinary Theoretical and Mathematical Sciences Program), Japan. The MOU with YITP, Japan was renewed in August, 2023. A full list of foreign institutions that the NCTS has set up partnership agreements with can be found on the NCTS webpage (http://www.phys.ncts.ntu.edu.tw/en/300/page302).

CECAM (Centre Européen de Calcul Atomique et Moléculaire) was established in 1969 to promote fundamental research on advanced computational methods, and its Headquarter is currently located in Lausanne, Switzerland. Academia Sinica (AS) became its 29th member with a MOU last year. AS and NCTS as well as other Taiwanese institutions are forming a CECAM-TW node, and a MOU between the CECAM-TW node and CECAM is expected to sign this November. A "kick-off" workshop will be held in Taiwan in the second half of 2025, and many of our TGs will be in a good position to integrate some of the TG events to either adapt a CECAM form or to draw support from CECAM.

India is a vast country in terms of land, population and science, and yet NCTS has no academic partnership there. Thus, to promote collaboration and cooperation with Indian institutions, we have been approaching our Indian friends and colleagues. As a result, an MOU of the NCTS Physics with S. N. Bose National Centre for Basic Sciences, Kolkata, India, is being discussed, and hopefully will be signed in the near future. We will continue striving to forge new cooperation agreements with more international institutions.

We have constantly promoted the academic exchange and collaboration with the overseas institutions with which we have signed an

MOU. In particular, NCTS Physics and KIAS (Korean Institute for Advanced Study) signed an MOU already in 2000, in order to promote and develop cooperation in the field of physical sciences between the two institutions. Since then, the two Institutions have organized many joint activities especially in the field of high energy physics, before the COVID-19 pandemic. Since the COVID-19 pandemic was leaving us in late 2022, we organized the first joint NCTS-KIAS workshop in the fields of condensed matter and materials physics in the NCTS in April last year (Fig. B4.2). Eighty people from both Korean and Taiwan participated the joint workshop. The second joint NCTS-KIAS workshop was held in April this year in KIAS, Seoul, Korea. Also, we held the inaugural NCTS-iTHEMS Joint Workshop on from Matters to Spacetime: Symmetries and Geometry in the NCTS last month (see https://www.phys.ncts.ntu.edu.tw/act/actnews/NCTS-58162719/home/introduction).

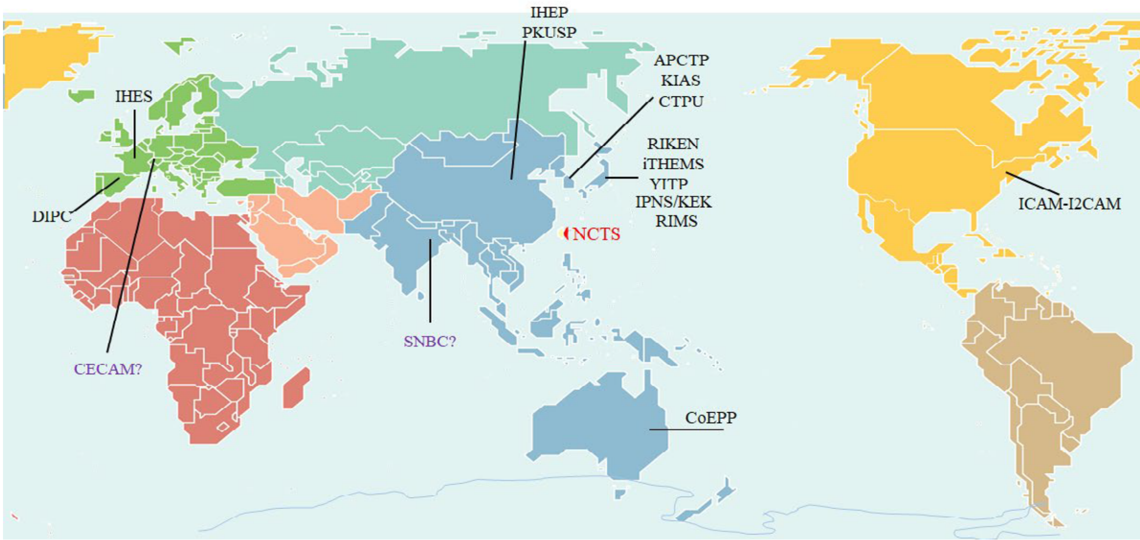


Fig. B4.1 Geographic locations of fourteen academic institutions with which NCTS Physics has signed an MOU. A CECAM-TW node with CECAM, located in Switzerland, will be signed soon. An MOU of NCTS Physics with S. N. Bose National Centre for Basic Sciences (SNBC) is being discussed.

Fig. B4.2 Photo taken during the 2023 NCTS-KIAS Workshop on Ab Initio Approaches to Quantum Materials, April 27-29, in the NCTS.

Overseas visitors: NCTS has played an important role in promoting academic exchange and collaboration with researchers worldwide. Since Jan., 2021, NCTS Physics has received overseas visitors of about 530 person-times in total. Many of our visitors were not supported by the Division. They included distinguished scientists such as Academicians Nai-Chang Yeh (CalTech), Steven Louie (UC Berkeley) and Dam Thanh Son (U. of Chicago) who came to give a lecture or seminar to us. Most of the visitors are short-term visitors, staying up to 7 days, although quite a few visitors spent more than two weeks here.

C. Financial Report

C.1 Statistical Data of NSTC Budget, Universities Matching Funds and Balance

Expenditure of Year 2023

For year 2023, we received 39+4M from NSTC, slightly above that (40M) of the first year, and 15.6+1.6M matching fund from NTU (40 % of NSTC funding). Note that the additional funding of 4M was allocated by the NSTC to our Division in July and as a result, NTU also increased its matching fund by 1.6M. In Phase V of NCTS, Physics Division set up four Hubs, two in Hsinchu (NTHU, NYCU), one in Tainan (NCKU) and one in Kaohsiung (NSYSU). According to the mutual agreement among the NSTC, NTU and Hub-hosting universities, NTU would transfer up to 40 % of the NSTC funding to the Hub-hosting universities to support the operation of the Hubs. In return, the four universities would offer matching funds of 25 % of the funding they receive from NTU. Therefore, all together we had a total of about 64.2 M funding available for the Division operations in 2023.

The usage of the funding was about 99 % in 2023. A major part of the expenditure is on the salary of the research staff (postdocs and research assistants). Another main spending is the operational cost of the center and hubs. This was then followed by the budget for supporting academic activities. Note that several M was spent each year to support international travels and the priority is given to young researchers, students, postdocs and junior faculty members.

Expenditure of Year 2024 (as of 9/30)

We received 39 from NSTC and 15.6 matching fund from NTU (40 % of NSTC funding) this year. The four Hub-hosting universities also offer their matching funds (25 % of the funds they receive from NTU). This resulted in a total of 58.5M to the Division for the operations in 2024.

About 56 % of the combined funding (total 58.5M) has been used so far this year. Since the 2024 NCTS Physics Grant (4/5) has been extended to the end of March, 2025, we thus project the total expenditure of the year until the end of next March and find that by that time, the usage rate would be 95 %.

C.2 Host University (NTU)'s Commitment

The NCTS Physics gratefully acknowledges the support and matching fund offered by the National Taiwan University in the past two years, which has been the other major resource for the NCTS. The host university commitment by NTU has been well delivered so far, as promised in the NTU proposal. There are three categories to describe. First of all, the

Division appointed 30 CSs in 2023 and 2024. However, the NSTC only allocates the salaries for 20 CSs each year. Thus, NTU has offered salaries for seven Center Scientists in the Physics Division in the past two years. NTU has also committed several quotas of postdoctoral salaries for the Division. Such personnel matching fund helps to make the NCTS to be more like a half-solid center, based not only on the NSTC project money but also on the host university commitment, hence contributing to a more stable environment for advanced research. Furthermore, the NCTS somehow is not allowed to use the NSTC funding to pay the travel expenses of the overseas postdocs when they first come to work in the Center. Consequently, these travel expenses have all been covered by the NTU matching fund. The salaries of some research assistants and administrative staff have also been covered by the NTU matching fund.

Secondly, NTU has provided money for activities operated by NCTS Thematic Groups, especially in the Thematic Groups based in the Center. Thirdly, NTU has provided equipment budget not only for desktop computers and laptop computers but also for mediate size PC clusters with both CPU and GPU nodes for the Center's postdocs and scholars to use. NTU has also paid for computer software, construction and maintenance of the Divisional website. Fourthly, NCTS Physics Division occupies the third and fourth floors in the Chee-Chun Leung Cosmology Hall. While NTU offers the fourth floor to the Physics Division for free, the third floor was rent to the Division by the Leung Center for Cosmology and Particle Astrophysics. NTU covered the rent for the third floor (about 2.75M for 2023 and 2024). Other support includes: guest houses, sport facilities and libraries etc. for the NCTS postdocs and also long-term or short-term visitors.

C.3 Hub Universities (NTHU, NYCU, NCKU and NSYSU)' Contributions

NCTS Physics also acknowledges the support and matching fund from the four Hub hosting universities (NTHU, NYCU, NCKU, NSYSU), which consists of additional resources for the Physics Division. Their commitments have also been rather well delivered in the past two years. For example, the Hub hosting universities provide the office space for their respective CSs and postdocs as well as administrative assistants. As mentioned above, the Division appointed 30 CSs in 2023 and 2024, while the NSTC only allocates the salaries for 20 CSs each year. Hubs offer the salaries for quite a few CSs in the past two years.

II. Highlights of the Thematic Group Program

Thematic Group 1.1 Quantum Computing and Interdisciplinary Applications

Coordinator: Hsi-Sheng Goan (National Taiwan University; Email: goan@phys.ntu.edu.tw)

I. Brief Description

Quantum computing leverages the principles of quantum mechanics to process and manipulate information in ways that are fundamentally different from classical computing. This enables the potential for solving complex problems that are currently intractable with classical computers. As quantum computing continues to advance, it is crucial for researchers and practitioners to collaborate across disciplines to harness its potential for solving real-world problems. Quantum computing and its interdisciplinary applications represent an exciting and rapidly evolving field at the intersection of physics, computer science, and engineering.

Thus, the core members of the Thematic Group 1.1 are composed of a team of established researchers and outstanding young scientists with diverse backgrounds and disciplinaries. The coordinator of TG 1.1 is Hsi-Sheng Goan (NTU)-Physics), and the core members are Hao-Chung Cheng (NTU-Electrical Engineering), Chiao-Hsuan Wang (NTU-Physics), Yuan-Chung Cheng (NTU-Chemistry), Jie-Hong Jiang (NTU-Electrical Engineering), Jyh-Pin Chou (NTU-Graduate School of Advanced Technology), and Yao-Hsin Chou (National Chi Nan University-Computer Science). Currently, TG1.1 has two postdocs, Dr. Shih-Kai Chou, and Dr. Jebarathinam Chellasamy and one full-time research assistant, Mr. Yu-Chao Huang.

The research topics of TG1.1 focus on quantum computing and its various applications, including quantum circuit synthesis and compilations, quantum error mitigation and correction, quantum dynamics and simulations, quantum computational chemistry and bioscience, Quantum machine learning, quantum finance and optimization problems, quantum sensing and metrology, and quantum communication theory and protocols.

II. Activities

TG1.1, TG1.2 & TG1.3 have a consensus to jointly plan and co-organize academic activities, such as workshops, conferences, short-term schools, and training courses, related to quantum computing and quantum information. We summarize below the events primarily organized by TG1.1.

TG 1.1 holds regular weekly seminars as well as special seminars co-organized jointly with the Center for Quantum Science and Engineering (CQSE) at NTU during the semesters. TG1.1 organized the Joint NCTS Phys-Math Summer School on Quantum Information from June 25-27, 2024. This event aimed to bring the physics and mathematics students and researchers together to learn and interact from different perspectives among one another. TG1.1 co-organized the 1st Joint Symposium on Quantum Computing held in Seoul, Korea from August 24–25, 2023 and the 2nd Joint Symposium on Quantum Computing at NTU, Taipei, Taiwan from August 22–24, 2024 with participants from Japan, Korea, Czech Republic, US, Singapore, Taiwan. TG1.1 also helped co-organize the 27th Annual Conference on Quantum Information Processing (QIP) held in Taipei, Taiwan from January 13-19, 2024. The QIP is one of the most prestigious international conferences in the field of theoretical quantum information science. Center scientists Hao-

Chung Cheng and Hsi-Sheng Goan are two of the main organizers of the conference. More than 700 researchers and students around the world in the field of quantum information science participated in the QIP 2024 conference

III. Visitors and International Collaborations

International collaborations:

1. Prof. Sun-Yuan Kung, Dept. of Electrical Engineering, Princeton University, USA
2. Prof. Seigo Tarucha, RIKEN, Japan
3. Prof. Andrew Dzurak and Dr. Chih-Hwan Henry Yang, UNSW, Australia
4. Prof. Alice Hu, Department of Mechanical Engineering, City University of Hong Kong, Hong Kong.
5. Dr. Tanmay Singal, Institute of Physics, Nicolaus Copernicus University, Poland
6. Dr. Samuel Yen-Chi Chen, Wells Fargo, New York, NY, USA
7. Prof. Viðar Guðmundsson, University of Iceland, Iceland.

Visitors:

1. Prof. Tzu-Chieh Wei (魏子傑) from the C.N. Yang Institute for Theoretical Physics and Department of Physics and Astronomy, State University of New York at Stony Brook visited TG1.1 at NCTS-Physics Division from July 31 to August 9, 2023. During his visit, Prof. Wei delivered a seminar "Simulating large-size quantum spin chains on cloud quantum computers."
2. There were many overseas visitors coming to give seminars: Dr. Maud Vinet (Quobly), Prof. Viðar Guðmundsson (University of Iceland), Prof. Tetsufumi Tanamoto (Teikyo University), Dr. Kevin Sung (IBM), Prof. Dominik Zumbühl (University of Basel), Dr. Hsin-Yuan Huang (Google Quantum AI, MIT & Caltech), Dr. Chih-Hwan Henry Yang (UNSW), Mr. Chi-Fang Chen (Caltech), Prof. Aurel Gabris (Czech Technical University in Prague), Prof. Jung-Tsung Shen (Washington University in St. Louis), Prof. Bei Zeng (Hong Kong University of Science and Technology), Tony Jin (Université Côte d'Azur), Prof. Jean-François Roch (Quantum-Saclay, Université Paris-Saclay).

IV. Highlights of Research Results

1. Boolean Matching Reversible Circuits: Algorithm and Complexity

Boolean matching is an important problem in logic synthesis and verification. Despite being well-studied for conventional Boolean circuits, its treatment for reversible logic circuits remains largely, if not completely, missing. This work provides the first such study. Given two (black-box) reversible logic circuits that are promised to be matchable, we check their equivalences under various input/output negation and permutation conditions subject to the availability/unavailability of their inverse circuits. Notably, among other results, we show that the equivalence up to input negation and permutation is solvable in quantum polynomial time, while its classical complexity is exponential. This result is arguably the first demonstration of quantum exponential speedup in solving design automation problems. Also, as a negative result, we show that the equivalence up to both input and output negations is not solvable in quantum polynomial time unless UNIQUE-SAT is, which is unlikely. This work paves the theoretical foundation of Boolean matching reversible circuits for potential applications, e.g., in quantum circuit synthesis.

2. Multi-objectives quantum-inspired optimization applied on quantum circuit synthesis model

Quantum circuit synthesis aims to minimize circuit size and optimize performance. However, distinct gate libraries have their own objectives that need to be considered, such as quantum cost, gate count, gate depth, or T depth. In current technology, the T gate nearly dominates the circuit execution time. Therefore, reducing the T gates and T depths is the biggest concern in the Clifford+T gate library. Meanwhile, the overall circuit size will be affected due to concerns about the T depth. The multiple objectives in quantum circuit synthesis results are sometimes conflicting with each other. In this subproject, we propose a multi-objective quantum-inspired optimization technique employing the entanglement mechanism to deal with the conflicting goals in quantum circuit synthesis. The proposed multi-objective optimization technique can provide optimal solutions for different objectives. Then, the Pareto front is built, where the optimal solution on the Pareto front has at least one objective superior to each other. Furthermore, the quantum-inspired optimization can provide a general-purpose circuit synthesis model that can be flexibly applied across various gate libraries, allowing for tailored optimization of quantum cost to meet specific requirements.

3. Achievability for classical communication over quantum channels

In quantum information science, transmitting classical information over a noisy quantum channel is a foundational task. To protect the transmitted messages against potential quantum noise, we have developed a simple, effective, and physically implementable coding strategy based on the so-called pretty-good measurement. The approach sharpens and streamlines the previously known achievable error bounds. Moreover, the proposed technique does not rely on structural hypotheses of the underlying quantum channel, such as independent and identical noises, and hence it applies to general non-correlated or non-stationary quantum channels. The derived one-shot capacities for unassisted and entanglement-assisted classical communication over quantum channels are both the tightest heretofore. One-shot error bounds for various quantum network information-processing protocols are also covered in a unified manner. The established error bounds are tighter than previously known, and the derivation is simpler, technically innovative, and more conceptually intuitive. The strength, simplicity, and variability of the derived error characterizations make the proposed coding and analysis likely a textbook approach when studying classical communication in one-shot and asymptotical quantum information theory. The established decoding technique to is expected to yield further applications in other fields of quantum information and technology.

4. Discrimination of Quantum States Under Locality Constraints in the Many-Copy Setting

Discriminating and testing entangled quantum states under quantum operations with locality constraints is one of the most technical challenging problems in quantum information science and quantum networking. We propose a mathematical framework to address this question and establish tight exponential error bounds for testing arbitrary *multipartite entangled pure quantum state* against its orthogonal complement. The contributions include investigating asymptotic inclusion relations between three important quantum operation classes – Local Communication with Classical Communication (LOCC), Separable (SEP) operations, and Positive Partially-Transposed (PPT) operations. Second, a novel measure was proposed to quantify the *unextendibility* of a product basis and we established its *multiplicativity* property. This mathematical technique yields a quantitative proof for a remarkable result: Tensor product of unextendible product bases (UPB) is still an UPB. Based on this, we demonstrated an *infinite separation* between the SEP and PPT operations by an example constructed from UPBs. This finding demonstrates an even more striking and counter-intuitive phenomenon because there is no entanglement involved in the UPB example, yet SEP could be substantially restricted compared to the PPT class.

5. Quantum capacities of transducers

We focus on developing protocols for hybrid quantum systems via quantum transduction, which is critical for building scalable quantum communication networks. A key contribution is the establishment of a generic formalism for quantum transduction across multiple platforms, including microwave-to-optical and optical-to-optical systems. We introduced a single metric based on quantum capacity to quantify the performance of quantum transducers, providing a framework for optimizing communication protocols. These advancements align closely with Taiwan's strategic goals in quantum information science, contributing to the development of quantum communication infrastructure.

6. Error-correction codes and fault-tolerant quantum computation

We have also shown that every quantum error-correcting code, including Pauli stabilizer codes and subsystem codes, has a similar structure, in that the code can be stabilized by commutative "Paulian" operators which share many features with Pauli operators and which form a Paulian stabilizer group. In addition, for the problem on counting stabilizer codes for arbitrary dimension, we have computed the number of $[[n, k]]_d$ stabilizer error-correction codes made up of d-dimensional qudits, for arbitrary positive integers d.

7. Efficient Quantum Simulation of Open Quantum System Dynamics on Noisy Quantum Computers

We have investigated characteristics of gate errors in IBM-Q quantum devices, and discovered that by designing dynamically-decoupled gate sequences (decoherence-inducing gates), random quantum noises can be generated on IBM-Q systems. We further employed such tailored decoherence-inducing gates to simulate energy transfer dynamics in a molecular dimer across coherent-to-incoherent regimes, and verified that the quantum simulation results are in good agreement to those of a numerically-exact classical method. Thus, we have shown that unwanted quantum noises could be turned into useful quantum resources. This new concept provides a new direction for quantum advantage in the NISQ era,

8. Accurate and efficient quantum computations of molecular properties

Quantum computational chemistry is one of the most promising target applications of near-term quantum computers, yet the small size and significant noise levels of nowadays quantum computers critically hamper its practicality. We have investigated several numerical methods for qubit number reduction and quantum circuit optimization for quantum computations of molecular energies and vibrational frequencies. Specifically, we have developed a novel method utilizing Daubechies wavelet molecular orbitals to make quantum chemistry calculations in quantum computers more efficient. This method was applied to show that quantum computation can be used to obtain vibration frequencies of diatomic molecules that are in excellent agreement with experimental results. Later, the same team showed that the Daubechies wavelet method can be extended to incorporate an efficient activate space selection scheme and the quantum variation eigensolver method to predict vibrational frequencies for a large database of diatomic molecules. This is the first time that a quantum computing method was benchmarked against a large dataset of experimental data, providing important information on the applicability of quantum computing methods for molecular property problems.

9. Quantum Machine Learning

Loading data into a quantum system is a crucial procedure in most quantum machine learning algorithms. How to efficiently implement it is largely open. We propose an algorithm based on quantum autoencoders to efficiently implement data loading. Further, by conducting numerical simulations, our method outperforms all the existing methods.

V. (Selected) Publications (with NCTS as an

affiliation only)

1. **Hao-Chung Cheng**, Andreas Winter, and Nengkun Yu, "Discrimination of Quantum States Under Locality Constraints in the Many-Copy Setting," Commun. Math. Phys. **404**,151 (2023).

2. **Hao-Chung Cheng**, "Simple and Tighter Derivation of Achievability for Classical Communication Over Quantum Channels," *PRX Quantum* **4**, 040330 (2023).

3. T. Singal, C. Chiang, E. Hsu, E. Ki, **Hsi-Sheng Goan**, and Min-Hsiu Hsieh, "Counting stabilizer codes for arbitrary dimension", Quantum **7**, 1048 (2023).

4. J.-Y. Kao and **Hsi-Sheng Goan**, "Existence of Pauli-like stabilizers for every quantum error-correcting code", Phys. Rev. A **108**, 032414 (2023).

5. S.-K. Chou, **J.-P. Chou**, A. Hu, **Y.-C. Cheng**, and_**Hsi-Sheng Goan**, "Accurate Harmonic Vibrational Frequencies for Diatomic Molecules via Quantum Computing", PRR **5**, 043216 (2023).

6. S.-Y. Kuo, Y.-C. Jiang, C.-Y. Hua, **Yao-Hsin Chou**, and S.-Y. Kuo, "Evo-Panel: Dynamic Visualization Tool for Optimization Process," *IEEE Trans. Emerg. Top. Comput.,* **7**, 1717 (2023).

7. S.-Y. Kuo, K.-C. Tseng, C.-C. Yang, and **Yao-Hsin Chou**, "Efficient Multiparty Quantum Secret Sharing Based on a Novel Structure and Single Qubits," *EPJ Quan. Technol.* **10**, 29 (2023).

8. S.-Y. Kuo, F.-H. Tseng, and **Yao-Hsin Chou**, "Metaverse Intrusion Detection of Wormhole Attacks based on a Novel Statistical Mechanism," *Future Gener. Comput. Syst.*, **143**, 179 (2023).

9. S.-Y. Kuo, K.-C. Tseng, **Yao-Hsin Chou**, and F.-H. Tseng, "Quantum Oblivious Transfer with Reusable Bell State," *Computers, Materials & Continua* **74**, 915 (2023).

10. **Hao-Chung Cheng** and L. Gao, "Error Exponent and Strong Converse for Quantum Soft Covering," IEEE Trans. Inf. Theory **70**, 3499 (2024).

11. Y.-C. Shen, L. Gao, **Hao-Chung Cheng**, "Optimal Second-Order Rates for Quantum Soft Covering and Privacy Amplification," IEEE Trans. Inf. Theory **70**, 5077 2024.

12. C.-Y. Cheng, C.-Y. Yang, Y.-H. Kuo, R.-C. Wang, **Hao-Chung Cheng**, C.-Y. Huang, "Robust Qubit Mapping Algorithm via Double-Source Optimal Routing on Large Quantum Circuits," ACM T Quantum Comput. **5**, 20 (2024).

13. T.-F. Chen, **Jie-Hong R. Jiang,** Boolean Matching Reversible Circuits: Algorithm and Complexity. In Proc. ACM/IEEE Design Automation Conference (DAC) 2024

14. T.-F. Chen, C.-H. Liu, **Jie-Hong R. Jiang,** A Holistic Approach to Rotation Synthesis for Fault-Tolerant Quantum Computation, Proc. IEEE International Conference on Quantum Computing and Engineering (2024).

15. Y.-H. Wu*, L. C. Camenzind, A. Noiri, K. Takeda, T. Nakajima, T. Kobayashi, C.-Y. Chang, A. Sammak, G. Scappucci, **Hsi-Sheng Goan**, and S. Tarucha*, "Hamiltonian Phase Error in Resonantly Driven CNOT Gate Above the Fault-Tolerant Threshold", npj Quan. Info. **10**, 8 (2024).

16. V. Gudmundsson*, V. Mughnetsyan, **Hsi-Sheng Goan**, J.-D. Chai, N. R. Abdullah, C.-S. Tang, V. Moldoveanu, and A. Manolescu, Magneto-optical properties of a quantum dot array interacting with a far-infrared photon mode of a cylindrical cavity, Phys. Rev. B **109**, 235306 (2024)

17. C. Xu, Y.-C. Huang, J. Y.-C. Hu, W. Li, A. Gilani, **Hsi-Sheng Goan**, H. Liu, BiSHop: Bi-Directional Cellular Learning for Tabular Data with Generalized Sparse Modern Hopfield Model, Proc. of the 41st International Conf. on Machine Learning, PMLR 235:55048-55075, 2024.

18. S. Sun, L.-C. Shih, **Y.-C. Cheng**, Efficient Quantum Simulation of Open Quantum System Dynamics on Noisy Quantum Computers, *Phys. Scr.* **99**, 035101(2024)

Thematic Group 1.2 Quantum Physics and Engineering

Coordinator: Wen-Te Liao (National Central University; Email: wente.liao@g.ncu.edu.tw)

I. Brief Description

Quantum physics and quantum engineering encompass various promising platforms, including atom-molecular-optics (AMO), solid-state systems, nuclear magnetic resonance (NMR), and superconducting systems. A key area of focus is the study of light-matter interactions, which enables the preparation, manipulation, and detection of quantum phenomena. Quantum optics and coherent quantum control are pivotal in advancing experimental quantum science. In Taiwan, researchers are actively involved in several key areas, such as: Photonic quantum state generation and detection; Quantum memory using light-atom interactions; Circuit-QED with Josephson junctions; Quantum gases in Bose-Einstein condensates; Precision spectroscopy with atoms and ions. In the context of quantum physics and quantum engineering, the following subjects are expected to be of growing importance in the coming decades:

1. **Quantum Optics**: Linked to quantum information processing
2. **Quantum Gases**: Related to many-body physics and quantum simulation
3. **Cavity and Circuit-QED, and Quantum Interfaces**: With implications for quantum computing
4. **Quantum-Assisted High-Precision Measurements and Quantum Metrology**.

II. Activities

In 2023-2024, we have held five activities including one international conference, two workshops, and two AMO summer schools:

1. 3rd TLL Workshop "Coherent Optical Control of Atomic Systems", November 8-10, 2024, Kaohsiung.

2. 2024 AMO Summer school, August 12-15, 2024, NTU Taipei.

3. 2023 AMO Summer school, August 22-25, 2023, AIDC Taichung.

4. 2nd TLL Workshop "Coherent Optical Control of Atomic Systems", July 6-8, 2023, Vilnius.

5. 17th International Conference on Squeezed States and Uncertainty Relations (ICSSUR), June 26-30, 2023, Taipei.

We would like to emphasize that since 2004, the original AMO Focus/Thematic Group has organized an annual summer school to support the entire AMO (Atomic, Molecular, and Optical) physics community in Taiwan. To enhance student training, most of the invited speakers are from local institutions, covering a wide range of AMO topics, including: cold atoms, quantum optics, attosecond and high-field physics, laser spectroscopy, atomic theory, precision measurement, and Quantum control so on. This comprehensive approach ensures that students gain exposure to key areas within the field.

III. Visitors and International Collaborations

Gediminas Juzeliūnas, Vilnius University, Vilnius, Lithuania

Julius Ruseckas, Vilnius University, Vilnius, Lithuania

Mārcis Auziņš, University of Latvia, Riga, Latvia

Teodora Kirova, University of Latvia, Riga, Latvia

I-Kang Liu, Newcastle University, Newcastle upon Tyne, UK

Ian B. Spielman, Joint Quantum Institute, Maryland, USA

Thomas Busch, Okinawa Institute of Science and Technology, Okinawa, Japan

Síle Nic Chormaic, Okinawa Institute of Science and Technology, Okinawa, Japan

Giedrius Žlabys, Okinawa Institute of Science and Technology, Okinawa, Japan

Zheng Li, Peking University, Beijing, China

Luqi Yuan, Shanghai Jiao Tong University, Shanghai, China

IV. Highlights of Research Results

Prototype of a phonon laser with trapped ions: Phys. Rev. Research 5, 023082 (2023).

The first author Chen-Yu Lee of this paper won the 2024 NCTS Student Outstanding Paper Award. This paper introduces a prototype of a tunable phonon laser using a large array of trapped ions, where optical tweezers are utilized to isolate a subset of ions, forming an acoustic cavity resonator for phonon lasing. The cavity loss can be dynamically controlled by adjusting the strength of the tweezers and the number of pinned ions, providing significant flexibility in manipulating the system's parameters. A blue-sideband transition is employed, generating the phonon laser through a mechanism similar to that of a Raman laser, where coherent energy transfer occurs between the internal states of ions and their vibrational motion, driving the phonon lasing process. The study delves deeply into the lasing dynamics, examining key aspects such as threshold behavior, population distribution within the cavity, second-order coherence, and linewidth narrowing. These parameters are essential for understanding and optimizing the performance and stability of the phonon laser. Additionally, the system supports multimode resonators, where mode competition is observed, allowing for different modes to stably coexist under certain conditions, depending on the initial configuration. This versatile platform provides new opportunities for exploring quantum interactions in phonon systems, advancing phonon-mediated quantum computing, communication, and precision metrology. The tunability and scalability of the system mark a significant step forward in the development of practical quantum technologies.

Synthetic Landau levels and robust chiral edge states for dark-state polaritons: Phys. Rev. Research 5, L042029 (2023).

The first author Yu-Hung Kuan of this paper won the 2024 NCTS Student Outstanding Paper Award. The discovery of quantum Hall effects has led to significant advancements in generating synthetic gauge fields for electrically neutral particles, which do not naturally experience the Lorentz force. Key implementations include ultracold atoms, photons, and electronic circuits. Among photonic systems, electromagnetically induced transparency (EIT) has drawn considerable attention, especially for its role in producing slow and stationary light in continuum media. EIT gives rise to neutral quasiparticles called dark-state polaritons (DSPs). We demonstrate an optical method for generating Landau levels and robust chiral edge states for DSP atomic coherence in a lattice-free medium. This approach generates synthetic gauge fields in the static laboratory frame, avoiding issues linked to mechanical rotation, such as excitations and destabilization. The lattice-free platform also allows easier interaction with Rydberg EIT and offers dynamic control, unlike static photonic structures. This system can rapidly control photonic flow, similar to a circuit, and holds the potential for simulating charged particles in magnetic fields, exploring nonlinear optics, negative-mass dynamics, and non-Hermitian quantum mechanics

V. (Selected) Publications (with NCTS as an affiliation only)

I. G. N. Y. Handayana, C.-C. Wu, S. Goswami, Y.-C. Chen, and H.-H. Jen, “Atomic excitation trapping in dissimilar chirally coupled atomic arrays,” Phys. Rev. Research 6, 013320 (2024).

C. G. Feyisa and H.-H. Jen, “A photonic engine fueled by entangled two atoms,” New J. Phys. 26, 033038 (2024).

C.-H. Chien, S. Goswami, C.-C. Wu, W.-S. Hiew, Y.-C. Chen, and H.-H. Jen, “Generating graph states in an atom-nanophotonic interface,” Quantum Sci. Technol. 9, 025020 (2024).

S.-H. Chung, I. G. N. Y. Handayana, Y.-L. Tsao, C.-C. Wu, G.-D. Lin, and H.-H. Jen, “Steady-state phases and interaction-induced depletion in a driven-dissipative chirally-coupled dissimilar atomic array,” Phys. Rev. Research 6, 023232 (2024).

T. Hsu, K.-T. Lin, G.-D. Lin, “Cooperative states and shift in resonant scattering of an atomic ensemble,” New J. Phys. 26 053026 (2024).

C.-C. Wu, K.-T. Lin, I. G. N. Y. Handayana, C.-H. Chien, S. Goswami, G.-D. Lin, Y.-C. Chen, and H.-H. Jen, “Atomic excitation delocalization at the clean to disordered interface in a chirally-coupled atomic array,” Phys. Rev. Research 6, 013159 (2024).

P. A.-Martinez, T. Forrer, D. Mills, JYW, L. Henaut, K. Yamamoto, M. Murao, and R. Duncan, “Distributing circuits over heterogeneous, modular quantum computing network architectures,” Quantum Sci. Technol. 9, 045021 (2024).

G. Biswas, S.-H. Hu, J.-Y. Wu, D. Biswas, D. and A. Biswas, “Fidelity and entanglement of random bipartite pure states: insights and applications,” Physica Scripta 99(7), 075103 (2024)

V. Kudriašov, W.-T. Liao, G. Juzeliūnas, H. R. Hamedi, "Spatially distributed PT symmetric refractive index using four-wave-mixing in a double-Lambda setup," Optics & Laser Technology 175, 110733 (2024).

J.-Y. Wu, K. Matsui, K., T. Forrer, A. Soeda, P. Andrés-Martínez, D. Mills, L. Henaut, and M. Murao, “Entanglement-efficient bipartite-distributed quantum computing with entanglement-assisted packing processes,” Quantum 7, 1196 (2023).

C.-Y. Lee, K.-T. Lin, and G.-D. Lin, “Prototype of a phonon laser with trapped ions,” Phys. Rev. Research 5, 023082 (2023).

A. K. Madhu, A. A. Melnikov*, L. E. Fedichkin, A. Alodjants, and R.-K. Lee, "Quantum walk processes in quantum devices," Heliyon 9, e13416 (2023).

A. Melnikov, M. Kordzanganeh, A. Alodjants, and R.-K. Lee, "Quantum Machine Learning: from physics to software engineering," Advances in Phys. X (Review Article) 8, 2165452 (2023).

J.-H. Chang, C.-Y. Lin, and R.-K. Lee, "Interplay between intensity-dependent dispersion and Kerr nonlinearity on the soliton formation," Opt. Lett. 48, 4249 (2023).

Y.-C. Wang, H.-H. Jen, and J.-S. You, “Scaling laws for non-Hermitian skin effect with long-range couplings”, Phys. Rev. B 108, 085418 (2023).

Y.-C. Wang, K. Suthar, H.-H. Jen, Y.-T. Hsu, and J.-S. You, “Non-Hermitian skin effects on thermal and many-body localized phases”, Phys. Rev. B 107, L220205 (2023).

X. Wang, Y.-H. Kuan, J. J. Cui, Y. K. Yang, F. X., W.-T. Liao, L. Yuan, Y. Cheng, Z. Liao, Z. Li, and S. B. Zhang, "Propagation effects of seeded collective emission by two-photon excited oxygen atoms" Phys. Rev. Research 5, 043293 (2023).

Y.-H. Kuan, S.-Y. Lee, S.-W. Shao, W.-C. Chiang, I-K. Liu, J. Ruseckas, G. Juzeliūnas, Y.-J. Lin, W.-T. Liao, "Synthetic gauge potentials for the dark state polaritons in atomic media" Phys. Rev. Research 5, L042029 (2023).

Thematic Group 1.3 Quantum Information and Communication

Coordinator: Hong-Bin Chen (National Cheng Kung University; Email: hongbinchen@gs.ncku.edu.tw)

I. Brief Description

Quantum information science (QIS) is a thriving, multidisciplinary research area that has attracted the interest of experts worldwide from physics, mathematics, computer science, information theory, etc. A primary goal of the research program is to harness features unique to quantum systems to perform tasks that are otherwise impossible or could only be performed much less efficiently. In recent years, tremendous progress has been made in our ability to prepare, manipulate, and control quantum systems, thus paving the way to experimentally realizing many of the splendid theoretical proposals. Yet, obstacles remain to be overcome, and our understanding of the implications of the underlying physical theories is still limited.

The primary mission of TG 1.3 is thus to provide a platform to facilitate communications and discussions among researchers working in these areas in Taiwan, to make solid progress in advancing our understanding and devising/realizing applications thereof. Through this platform and the organized activities, we hope to enhance collaborations among domestic scholars and provide opportunities for them to connect with international links. In the past two years, our core members have focused on the following research subjects

(1) Information-theoretic approaches to physics.
(2) Quantum communications and quantum cryptography.
(3) Quantum dynamics in open quantum systems.
(4) Beyond conventional quantum theory.
(5) Characterization, certification, and distillation of quantum resources

II. Activities

In the past two years, TG 1.3 held three series of activities.

The first series is the Workshop on Quantum Science and Technology. As early as 2004, several former members had organized the early edition of this event. Since 2017, our group members have begun to take on the organization of the workshop. Now this series has become one of the most important events focusing on quantum information science and quantum technologies in Taiwan. This series of workshops aims to bring together researchers working in quantum science & technology to (1) present their recent findings and (2) promote research activities, interactions, and collaborations among the participants.

The second one is the series of the young researchers forum on QIS. This event is initiated since 2017. The early edition of this series aims to provide an opportunity for young researchers, including newly hired faculties, postdocs, and graduate students, to present their findings, and to make new connections at an early stage of their research career. In the recent two years, this series was further promoted to an international version. In February 2023, we have co-organized this event with Prof. Andreas Buchleitner from Universität Freiburg. We have also invited 6 foreign speakers (mainly from Germany). In the same year, we have organized another international event, RIKEN-KAIST-NCTS Joint Workshop on QIS, with Prof. Joonwoo Bae from KAIS, Korea and Prof. Neill Lambert from RIKEN, Japan. During this event, we invited a total of 9 speakers from the three institutes. In October 2024, this international joint workshop was hosted by Prof. Joonwoo Bae at KAIST in

Korea. The agenda has been extended to two days and we have included more speakers from three institutes.

The third one is the gular Quantum Information Science (QIS) seminars every second Monday over lunchtime at the NCKU campus. These seminars are held during semester periods. These seminars are targeted primarily at graduate school students and are usually delivered by domestic experts in the field. Occasionally, we also have QIS seminars presented by visiting experts on other days of the week. From Jan 2021 to mid-September 2024, TG 1.3 has hosted a total of 76 QIS seminars at NCKU.

III. Visitors and International Collaborations

Konrad Banaszek, Uniwersytet Warszawski, Polska.
Andreas Buchleitner, Albert-Ludwigs-Universität Freiburg, Deutschland.
Max Masuhr, Universität Kassel, Deutschland.
Andrea Alberti, Max Planck Institute für Quantenoptik, Deutschland.
David Bustor, Lunds Universitet, Sverige.
Edoardo Carnio, Albert-Ludwigs-Universität Freiburg, Deutschland.
Giacomo Sorelli, Fraunhofer-Institut für Optronik, Deutschland.
Joonwoo Bae, KAIST, Korea.
Ashutosh Rai, KAIST, Korea.
Jiyoung Yun, KAIST, Korea.
Sung Won Yun, KAIST, Korea.
Kieran Flatt, KAIST, Korea.
John Martinis, UC Santa Barbara, USA.
Tzu-Chieh Wei, Stony Brook University, USA
Peter Sidajaya, National University of Singapore, Singapore.
Neill Lambert, RIKEN, Japan.
Paul Menczel, RIKEN, Japan.
Chung-Yun Hsieh, University of Bristol, UK.
Yink Loong Len, Yale-NUS College, Singapore.

IV. Highlights of Research Results

Quantum correlations and no-signaling correlations

Y.-C. Liang's group fully characterized when the boundary of the set of quantum correlations coincides with the boundary of the set of no-signaling correlations. They further showed that self-testing is possible in each Class of these common boundaries, even though many of these extremal correlations are geometrically non-exposed. They also attained a similar characterization for quantum correlations derived from finite-dimensional maximally entangled states. See Ref. [3].

Analog simulation approach on near-term quantum computers

Although still in an era of noisy intermediate-scale quantum (NISQ) devices, several proof-of-principle demonstration showcasing prominent breakthroughs of quantum computers outperforming conventional computers has been realized. H.-B. Chen’s group proposed to simulate the nonclassical free induction decay (FID) process of NV centers in diamond on IBM quantum computers. Their theoretical investigation pointed out that the nonclassicality of the FID process could be induced by several factors, including the strength of external magnetic fields, the polarization in the ambient nuclear spin bath, and the precession arrangement of the nuclear spin caused by both the external magnetic fields and the hyperfine interactions to the electron spin. Their simulations agreed with the theoretical investigations very well. Meanwhile, they also investigated the noise caused by the crosstalk between qubits and proposed an efficient way to suppress it. See Ref. [5].

Non-Hermitian Quantum mechanics

The Hilbert spaces for non-Hermitian quantum systems are known to be interesting because they require non-trivial metrics, which are closely related to quantum phase transitions.

Collaborating with researchers from Poland and Japan, C.-J. Ju and G.-Y. Chen derived the local curvatures of the Hilbert space bundles. They first derived the evolution equations for quantum states in parameter space via the general properties of the metrics. By further examining the equations, they found that the parameter space can be merged naturally into the Hilbert space bundle as emergent dimensions so that the local curvatures of the Hilbert space bundles can be obtained. Meanwhile, they also showed that many physical quantities are related to the emergent dimensions, including the Berry connections and the Berry curvatures. Moreover, the analytic form of fidelity susceptibility, which is often used to detect quantum phase transitions and exceptional points, can also be obtained using the evolution generator for the emergent dimension. Furthermore, they have also shown that the entanglement between qubits can be prolonged by the quantum effects of local surface plasma on a metallic nanoparticle. See Ref. [6].

Characterization of quantum temporal correlations

In Ref. [8], S.-L. Chen and his collaborator introduced a framework called *instrument moment matrices* (IMMs) to analyze quantum systems' behavior over time, particularly useful for situations where detailed knowledge of the devices involved is limited. This device-independent method allows researchers to measure temporal quantum correlations by preparing a quantum state, sending it through a channel, and remeasuring it. The flexibility of IMMs means it can adapt to different experimental constraints, like no-signaling rules (to prevent information leakage over time), dimensional limits, or rank restrictions on measurements. The IMM framework is significant for practical quantum applications, enabling researchers to measure critical temporal correlations and detect purely quantum behaviors even with minimal device details. For example, the framework can calculate upper bounds on violations of temporal Bell inequalities—similar to spatial Bell inequalities, which reveal quantum characteristics not possible in classical systems. IMMs also aid in measuring *temporal steerability*, where the correlations between different measurement times help confirm quantum behaviors. Another application is optimizing quantum randomness access codes, where quantum systems improve the probability of accurately transmitting bits of information compared to classical methods. This work extends to complex quantum setups, supporting various needs in emerging technologies like secure quantum communication and quantum randomness generation. Ultimately, IMMs bridge the gap between fully detailed device specifications and general, device-independent methods, making them valuable in advancing secure, practical quantum systems for real-world use.

Quick charging of quantum batteries

One of the core concepts of quantum mechanics is that matter also behaves as wave. Following this concept, any quantum particle can stay in a superposition state. By utilizing this superposition principle, Y.-N. Chen and his group members have developed a new approach, which can be used to charge quantum batteries faster than usual. A quantum battery can be modelled as a qubit, and the charging process is a kind of quantum dynamical process. By utilizing the approach of superposition of dynamical path, a quantum battery can be fully charged within a shorter time period than that without superposition technique. They have also simulated their approach on IBMQ and IonQ quantum computers to show the feasibility of this approach. This work has been highlighted as Editor's suggestion by APS. See Ref. [9].

Detecting quantum steering of states with machine learning approach

The characterization of the EPR steerability of a bipartite state is highly nontrivial due to the cumbersome optimization over all possible incompatible measurements. This is very different from the steerability of assemblages, which can be determined efficiently with the computational algorithm of semidefinite program. To address this issue, H.-B. Chen's group leveraged the power of the deep learning (DL) models to infer the hierarchy of steering measurement setting. A computational protocol consisting of iterative tests was constructed to overcome the optimization, meanwhile, generating the necessary training data. They showed that the well-trained deep learning model was capable of accurately predicting the minimum number of observables necessarily to demonstrate the EPR steerability. Meanwhile, with this DL approach, H.-B. Chen's group also identified an efficient approach characterizing the EPR steerability with Alice's ellipsoid. See Ref. [14].

V. (Selected) Publications (with NCTS as an affiliation only)

[1] Po-Chen Kuo, Neill Lambert, Mauro Cirio, Yi-Te Huang, Franco Nori, and Yueh-Nan Chen, *Kondo QED: The Kondo effect and photon trapping in a two-impurity anderson model ultra-strongly coupled to light*, Physical Review Research **5**, 043177 (2023).

[2] Po-Chen Kuo, Jhen-Dong Lin, Yin-Chun Huang, and Yueh-Nan Chen, *Controlling periodic Fano resonances of quantum acoustic waves with a giant atom coupled to a microwave wave guide*, Optics Express **31**, 42285 (2023).

[3] Kai-Siang Chen, Gelo Noel M. Tabia, Chellasamy Jebarathinam, Shiladitya Mal, Jun-Yi Wu, and Yeong-Cherng Liang, *Quantum correlations on the no-signaling boundary: self-testing and more*, Quantum **7**, 1054 (2023).

[4] Rivu Gupta, Saptarshi Roy, Shiladitya Mal, and Aditit Sen(De), *Emergence of monogamy under static and dynamics scenarios*, Physical Review A **108**, 012420 (2023).

[5] Yun-Hua Kuo and Hong-Bin Chen, *Adaptively partitioned analog quantum simulation on near-term quantum computers: The nonclassical free-induction decay of NV centers in diamond*, Physical Review Research **5**, 043139 (2023).

[6] Chia-Yi Ju, Adam Miranowicz, Yueh-Nan Chen, Guang-Yin Chen, Franco Nori, *Emergent parallel transport and curvature in Hermitian and non-Hermitian quantum mechanics*, Quantum **8**, 1277 (2024).

[7] Wan-Guan Chang, Chia-Yi Ju, Guang-Yin Chen, Yueh-Nan Chen, and Huan-Yu Ku, *Visually quantifying singe-qubit quantum memory*, Physical Review Research **6**, 023035 (2024).

[8] Shin-Liang Chen and Jens Eisert, *Semi-Device-Independently Characterizing Quantum Temporal Correlations*, Physical Review Letter **132**, 220201 (2024).

[9] Po-Rong Lai, Jhen-Dong Lin, Yi-Te Huang, Hsien-Chao Jan, and Yueh-Nan Chen, *Quick charging of a quantum battery with superposed trajectories*, Physical Review Research 6, 023136 (2024).

[10] Shounak Datta, Shiladitya Mal, Arun K. Pati, and A. S. Majumdar, *Remote state preparation by multiple observers using a single copy of a two-qubit entangled state*, Quantum Information Processing **23**, 54 (2024).

[11] Kai-Siang Chen, Shiladitya Mal, Gelo Noel M. Tabia, and Yeong-Cherng Liang, *Hardy-type paradoxes for an arbitrary symmetric bipartite Bell scenario*, Physical Review A **109**, 042206 (2024).

[12] Chung-Yun Hsieh, Gelo Noel M. Tabia, Yu-Chun Yin, and Yeong-Cheng Liang, *Resource Marginal Problems*, Quantum **8**, 1353 (2024).

[13] Li-Yi Hsu, *Nonlocal correlations in quantum networks distributed with different entangled states*, New Journal of Physics **26**, 033026 (2024).

[14] Hong-Ming Wang, Huan-Yu Ku, Jie-Yien Lin, and Hong-Bin Chen, *Deep learning the hierarchy of steering measurement settings of qubit-pair states*, Communications Physics **7**, 72 (2024).

[15] Chan Hsu, Yu-Chien Kao, Hong-Bin Chen, Shih-Hsuan Chen, and Che-Ming Li, *Photonics Non-Markovainity Identification by Quantum Process Capabilities of Non-CP* Advanced Quantum Technologies **7**, 2300246 (2024).

[16] Chung-Yun Hsieh and Shin-Liang Chen, Thermodynamics Approach to Quantifying Incompatible Instruments, Physical Review Letters **133**, 170401 (2024).

Thematic Group 2.1 High Energy Phenomenology

Coordinator: Cheng-Wei Chiang (National Taiwan University; Email: chengwei@phys.ntu.edu.tw)

I. Brief Description

The members of our TG focus on three main research topics: astroparticle physics, dark matter (DM) physics, flavor physics (including heavy quark systems and neutrino physics), and Higgs physics. We explore the possibility of discovering new physics at various frontiers (energy, precision, and cosmology), but also examine experimental data within the framework of the Standard Model. Within these two years, we have 22 active members affiliated with 10 different institutes and 2 postdocs stationed at the headquarters.

II. Activities

Our TG supports regular seminars at NTHU, NTNU and NTU. Such seminars bring latest developments in particle physics to the above-mentioned groups and stimulate new ideas among the audience.

On June 7-9, 2023, Prof. Anthony Francis co-organized with TG4.1 "The Future is non-perturbative" workshop at NTHU, inviting keynote speakers within Taiwan and from various countries (USA, Japan, Switzerland, Poland). This is a topical workshop on non-perturbative physics in high-energy physics and condensed matter systems. This and other contributions enabled us to host an international workshop with 56 participants and 6 international invited keynote speakers.

The workshop had strengthened the collaboration and dialogue within the field of particle physics and condensed matter physics locally and internationally at the same time.

On 8/21-25/2023, we hosted the 2023 Summer Institute in Sun-Link-Sea, with many invited speakers from different countries (Taiwan, Japan, Korea, USA, Australia, Germany, Morocco). As an activity that rotates among China, Japan, Korea, and Taiwan, participants of this School are able to exchange exciting ideas with other scholars in the East Asia region.

On 12/15-17, 2023, we had the Annual Theory Meeting: Particle Physics, String Theory, Cosmology, and Astrophysics, which aimed to bring together leading researchers from abroad to give research talks on specific themes, and local young researchers to share their work. This year's main focus was on recent progress in constraints on physics beyond the standard model, stemming from astro-physical observation and new generalized symmetries. There were so many participants from various countries filling the lecture hall (see the picture below).

On June 4-6, 2024, NTHU organized "The Future is Flavourful" workshop, one of the series that has been held in the Hsinchu area. This year's meeting focused on flavor physics, from the Standard Model flavors of neutrinos and quarks to potential new dark and exotic flavors beyond the Standard Model of particle physics. The aim was to promote young scientists and bridge gaps between various subfields. We have invited colleagues working on experimental aspects of flavor physics to gain a deeper understanding of what is currently being probed and what can be probed in the future.

On June 6/10-13, 2024, we hosted a new

workshop that involved different institutes from three different countries. The Japan-US-Taiwan Particle Physics Workshop was designed as a collaborative effort to pool and discuss novel ideas from particle physics, cosmology, and related experimental findings. We aimed to foster an interactive environment for participants to engage in discussions and exchange insights. The workshop is hosted by the NCTS and features significant contributions from KEK (High Energy Accelerator Research Organization), the University of Tokyo, and Florida State University. We are planning to continue this workshop every year, with the Yukawa Institute of Theoretical Physics possibly hosting the next one in 2025.

On Oct 21-24, 2024, we organized The Fifteenth Particle Physics Phenomenology (PPP15) Workshop. This workshop is a biennial meeting with a rich history dating back to 1992 (skipping only a few times due to incidents such as SARS and COVID), one of the most important gatherings in the particle physics community in Taiwan. The workshop serves as a vital platform for foreign and domestic scholars working on particle physics experiments and theories to share the latest experimental results and developments in various models or theoretical frameworks. It features comprehensive lectures on topics of current interest to the community, as well as shorter presentations on more specific applications. It aims to inspire innovative ideas and help form new collaborations among the participants.

This year, we invited three lecturers from the US to give pedagogical introductions to deep machine learning and its application in particle and astroparticle physics, light dark matter phenomenology, and effective field theory approach to SM and Higgs physics. The program has 33 speakers from various countries (China, Germany, Japan, Korea, Spain, Taiwan, and USA; see the group photo below).

All the participants have enjoyed the meeting and claimed to learn very much for each other's talks.

III. Visitors and International Collaborations

We have many visitors from abroad during these two years. Aside from those who visited NCTS just for meetings, we have the following visitors with longer stays:

- Hsin-Chia Cheng, UC Davis
- Yi Chung, Max Planck Institute, Heidelberg
- Ian Low, Northwestern University
- Takeo Moroi, University of Tokyo
- C.P. Yuan, Michigan State University

Various active members of our TG have international collaborations. Some of them are listed as follows:

Member	Countries of international collaborations
Chian-Shu Chen	Italy, Brazil, LVK (LIGO-Virgo-KAGRA) Collaborations
Chuan-Hung Chen	China
Cheng-Wei Chiang	Canada, China, Germany, Japan, Spain, USA
C.-J. David Lin	Germany, Japan, Poland, South Korea, Spain, UK, USA
Cheng-Pang Liu	China, India, Canada
Martin Spinrath	Germany, Indonesia, USA
Meng-Ru Wu	Denmark, Germany, Japan, USA

IV. Highlights of Research Results

Over the past two years or so, the research activities within our TG have been exceptionally productive, resulting in the publication of numerous works in leading journals. This output is a testament to the dedication and expertise of our members, who have consistently pushed the boundaries of their respective fields. Detailed information about these publications is provided at the end of this report.

Among the many achievements, we are particularly proud to highlight four significant publications in Physical Review Letters (PRL). These works exemplify the collaborative spirit that defines our group, as they were the result of successful partnerships between our Center Scientists and postdocs and international collaborators. We look forward to continuing this momentum in the coming years, further solidifying our reputation as a leading research group in the field.

Due to the space limit, we just highlight the results of the four PRL papers, although there are many other good works by members of our TG as well.

In PRL 130, no.11, 111002 (2023), Dr. Yen-Hsun Lin and Dr. Meng-Ru Wu along with their collaborators (including an experimentalist, Dr. Henry T.K. Wong) studied how light dark matter (DM) could be boosted by supernova neutrinos (SNν). The SNν boosted DM (BDM) arrives on Earth with time-of-flight (TOF) which depends only on the DM mass and is independent of the cross section. These BDMs can interact with detector targets in low-background experiments and manifest as afterglow events after the arrival of SNν. The characteristic TOF spectra of the BDM events can lead to large background suppression and unique determination of the DM mass.

In PRL 130, 141801 (2023), Dr. Hugues Beauchesne and Prof. Cheng-Wei Chiang found stringent bounds on the decay rate of the Higgs boson to a photon and a dark photon. For this decay to be potentially observable at the LHC, new mediators that communicate between the standard model and the dark photon must exist. They studied bounds on such mediators coming from the Higgs signal strengths, oblique parameters, electric dipole moment of the electron, and unitarity. The branching ratio of the process was constrained to be far smaller than the sensitivity of current collider searches, thus calling for a reconsideration of current experimental efforts. Because of this work, Dr. Beauchesne won the 2024 NCTS Postdoc Paper Award, and Prof. Chiang won the 2024 Sun Yat Sen Academic Research Achievement Award in Natural Sciences.

In PRL 131 (2023) 26, 261901, Prof. Jiunn-Wei Chen and his international collaborators reported a state-of-the-art lattice QCD calculation of the isovector quark transversity distribution of the proton in the continuum and physical mass limit using large-momentum effective theory. The result is non-perturbatively renormalized in the hybrid scheme with self renormalization which treats the infrared physics at large correlation distance properly, and extrapolated to the continuum, physical mass and infinite momentum limit. They also compare with recent global analyses for the nucleon isovector quark transversity distribution.

In PRL 133 (2024) 11, 111004, Dr. Yen-Hsun Lin and Dr. Meng-Ru Wu examined a novel component of diffuse contribution of supernova neutrino boosted dark matter and showed that this component could be probed by upcoming neutrino detectors like Hyper Kamiokande to set leading constraints on the properties of light dark matter. Besides, based on their continuous effort in studying the collective fast neutrino flavor conversions, they have recently proven that one can use an effective classical neutrino transport model based on the nature of scale separation and coarse-graining to robustly taking into account fast flavor conversions of neutrinos in supernova simulations. This is expected to have a ground-breaking impact and points to a realistic way going forward to address the consequence of neutrino flavor oscillations in supernova explosions, which is a long-standing missing piece of known physics in supernova theory.

As an example of cross-institute collaboration that was established in the capacity of NCTS, Prof. Chuan-Hung Chen at NCKU and Prof. Cheng-Wei Chiang at NTU have continued to work together on new physics models to explain various observed experimental anomalies, including the muon g-2, coherent neutrino-nucleus elastic scattering, B to Kνν anomaly, R(D) and R(D*) deviations, W mass anomaly, etc. Currently, they are also working with a Center postdoc on a new physics model.

Prof. Jiunn-Wei Chen at NTU, Prof. Cheng-Pang Liu at NDHU, and Dr. Henry T.K. Wong at AS have also continued their long-time collaboration in the research of inverse Primakoff scattering for axionlike particle (ALP) couplings. The ALPs can be produced in the Sun, and are considered viable candidates for the cosmological DM. They identified new inelastic channels of inverse Primakoff processes due to atomic excitation and ionization.

V. (Selected) Publications (with NCTS as an affiliation only)

2023

Phys. Rev. Lett. 130 (11), 111002, 2023.
Phys. Rev. Lett., 130 (14), 141801, 2023.
Phys. Rev. Lett. 131 (26), 261901, 2023.
Phys. Rev. D, 108 (1), 015018, 2023.
Phys. Rev. D, 107 (1), 016014, 2023.
Phys. Rev. D 108 (4), 043007, 2023.
Phys. Rev. D 108 (6), 063003, 2023.
Phys. Rev. D 108 (8), 083013, 2023.
Phys. Rev. D 108 (8), 083002, 2023.
Phys. Rev. D 107 (8), 083016, 2023.
Phys. Rev. D 108 (12), 123038, 2023.
JHEP 06, 069, 2023. [Erratum: JHEP 07, 169 (2023)].
JHEP 10, 170, 2023.
Phys. Lett. B 838, 137682, 2023.
Phys. Lett. B 843, 138027, 2023.
Eur. Phys. J. C 83, 7, 599, 2023.
Int. J. Mod. Phys. A 38, no.25, 2350139, 2023.

2024

Phys. Rev. Lett. 133, 11, 111004, 2024.
Phys. Rev. D 109 (4), 043024, 2024.
Phys. Rev. D, 109 (5), 055038, 2024.
Phys. Rev. D, 109 (5), 055040, 2024.
Phys. Rev. D, 109 (7), 073008, 2024.
Phys. Rev. D, 109 (7), 075004, 2024.
Phys. Rev. D, 109 (7), 075043, 2024.
Phys. Rev. D 109 (8), 083019, 2024.
Phys. Rev. D 109 (8), 083020, 2024.
Phys. Rev. D, 109 (10), L101304, 2024.
Phys. Rev. D, 109 (12), 123008, 2024.
Phys. Rev. C 110 (1), 015504, 2024.
JHEP 06, 164, 2024.
JHEP 02, 138, 2024.
JHEP 09, 139, 2024.
Prog. Part. Nucl. Phys. 137, 104107, 2024.
J. Phys. G, 51(8):085001, 2024.

Thematic Group 2.2 High Energy Theory

Coordinator: Yu-tin Huang (National Taiwan University; Email: yutin@phys.ntu.edu.tw)

I. Brief Description

TG 2.2 Focuses on the interplay between high energy, gravitational, cosmology and condense matter physics. In the past two years our center scientists have made progress in all areas in the above. Including center scientist **Chong-Sun Chu** and **Dimitrios Giataganas** as well as center post-doc **Himanshu Parihar**, has been collaborating on many work including **Finding new massless Lifshitz field theory for arbitrary anisotropy index z:**, Center scientist Prof. **Yu-tin Huang** collaborated with prof. **Katsuki Aoki** of Kyoto University, who visited and attended 14th Taiwan String Workshop organized by NCTS, to study the scattering amplitude of unstable particles and understand it's complex analytic properties as well as its implications for positivity bounds in general EFT. **Anomalous Thresholds for the S-matrix of Unstable Particles.** Core member **Pei-Ming Ho** has formed an outstanding research group with visiting professor **Hiraku Kawai**, working on a wide variety of topics including Hawking radiation, Trans-Planckian Physics and Matrix models. The group includes PhD student Henry Liao, Wei-Hsiang Shao, master student Cheng-Tsung Wang, Tin-Long Chau. Prominent results include: **Planckian physics comes into play at Planckian distance from horizon, Stringy effects on Hawking radiation and cosmological scenarios.**

Our center scientists have received multiple awards including [2024] National Sun Yat-sen Grant, Distinguished Young Professor. **(Dimitrios Giataganas)** [2023] elected Fellow from Taiwan Physics Society **(Yu-tin Huang)** [2022] NSTC Outstanding Research Award **(Yu-tin Huang)** [2022] Outstanding Scholar Award, Foundation for the Advancement of Outstanding Scholarship. **(Chong-Sun Chu)** [2022] 2022 Young Theorist Award NCTS (3 years duration). National Center for Theoretical Sciences. **(Dimitrios Giataganas)** [2021] Columbus Young Scholar Fellowship, National Science and Technology Council. (Ministry of Science), Taiwan, 2021--2026. (Dimitrios Giataganas)

Currently, there are roughly 15 graduate/undergraduate students under our CS and Core members, along with 7 post-docs (3NCTS+2 NTU+1 NTNU+ 1 CYCU+ 1 NSYSU) at either the center, or under CS or core member's grant. They actively participate in center activities, for example post-doc Jaydeep Kumar Basak (CYCU) give a talk at 2022 ATM, while Himanshu Parihar (NCTS) and Michele Santagata (NTU) presented at Taiwan String workshop (14th).

II. Activities

Our TG continued to host international conferences such as 13th and 14th Taiwan String Workshop, as well as annual theory meeting in 2022 and 2023. These meetings continue to serve as a plat-form for engagement between the local and international community and especially introduce Taiwanese young talents to our community. In 2024, we are expected to host two major events:

1. "**NCTS Annual Theory Meeting: Particle Physics, String Theory, Cosmology, and Astrophysics**", Conference, Dec-14/16 2022 NTU
2. "**13th Taiwan String Workshops**", Conference, Taipei, Taiwan, 22-23 December 2022.

3. "**14th Taiwan String Workshop**", Taipei, Taiwan, Taipei Session 10/30-11/02 Kaohsiung session 11/03-11/05 2023
4. "**NCTS Annual Theory Meeting: Particle Physics, String Theory, Cosmology, and Astrophysics**", Taipei, Taiwan, Dec-15/17 2023 NTU
5. "**2024 East Asia Joint Workshop on Fields and Strings**", Conference, Kaohsiung, Taiwan, 18-22 Nov., 2024
6. "**QCD Meets Gravity**", Conference, Taipei, Taiwan, Dec 9 to 13, **2024**

At the same time the TG has been continuing to fund local seminars at NTU and NSYSU.

III. Visitors and International Collaborations

Currently, collaborations within the TG have been relatively successful as previously mentioned. There are also international collaborations that are currently under individual CS or core members. These include

Yu-tin Huang (CS): with Jung-Wook Kim (Potsdam Max Plank Institute) on gravitational wave physics, Aaron Hillman (Caltech) Laurentiu Rodina (BIMSA) on S-matrix bootstrap, and Song He (ITP Beijing) on geometry of scattering amplitudes. Katuski Aoki (Kyoto Univ) on S-matrix of unstable particles.

Chong-Sun Chu (CS): with Rong-Xin Miao (Zhongshan University) on BCFT and properties of quantum blackholes

Dimitrios Giataganas (CS): with Vangelis Giantsos (Athens U.) on holographic observables.

Pei-Ming Ho (Core Member): Yosuke Imamura (Tokyo Institute of Technology) and Emil T Akhmedov (Moscow Institute of Physics and Technology) on properties of Hawking radiation, and Yuki Yokokura (Riken) on interior of quantum black holes.

Feng-Li Lin (Core Member): with Kilar Zhang (Shanghai University) on dark stars and gravitational waves.

Chia-Hsien Shen (Core Member): Zvi Bern (UCLA) Julio Parra-Martinez (UBC) Enrico Herrmann (UCLA) Oliver Long (Potsdam Max-Plank Institute) on post Minkowskian expansion of bi-nary dynamics, Benoît Assi (FermiLab), Andreas Helset (Caltech), Aneesh V. Manohar (UC, San Diego), Julie Pagès (UC, San Diego) on standard model effective field theory. Daniel Green and Yiwen Huang (UC, San Diego) on positivity bounds in cosmological correlators.

IV. Highlights of Research Results

New class of massless Lifshitz scalar field theory in (1+1)-dimension

Center scientist prof. Chong-Sun Chu and prof. Dimitrios Giataganas as well as center post-doc Himanshu Parihar has found a new class of massless Lifshitz scalar field theory in (1+1)-dimension with an arbitrary anisotropy index z is constructed. It is demonstrated that there is a continuous family of ground states with degeneracy parameterized by the choice of solution to the equation of motion of an auxiliary classical system. The quantum mechanical path integral establishes a 2d/1d correspondence with the equal time correlation functions of the Lifshitz scalar field theory. The entanglement measures are shown to satisfy the c-function monotonicity theorems. In order to match with the field theory result for the entanglement entropy, a z-dependent radius scale for the Lifshitz background was proposed. This relation is consistent with the z-dependent scaling symmetry respected by the Lifshitz vacuum. Furthermore, the time-like entanglement entropy is determined using holography. The result suggests that there should exist a fundamental definition of time-like entanglement other than employing analytic continuation as performed in relativistic field theory. (JHEP 05 (2024) 284)

Anomalous Thresholds for the S-matrix of Unstable Particles

Center scientist Prof. Yu-tin Huang collaborated with prof. Katsuki Aoki of Kyoto University, demonstrated that anomalous thresholds associated with UV physics are unavoidable for unstable particles. This is in contrast to stable particles, where the anomalous thresholds are due to IR physics, set by the scale of the external kinematics. As a result, any dispersive representation for the amplitude will involve contributions from these thresholds that are not computable from the IR theory, and thus invalidate the general positivity bound. Indeed using toy models, we explicitly demonstrate that the four-derivative couplings for unstable particles can become negative, violating positivity bounds even for non-gravitational theories. (JHEP 09 (2024) 45)

Reflected entropy and Markov gap in non-inertial frames

Center scientist Dimitrios Giataganas worked with previous core member Wen-Yu Wen (CYCU) and Jaydeep Kumar Basak, Sayid Mondal. They showed that reflected entropy between two modes of a free fermionic field degrades monotonically as a result of the Unruh effect, eventually reaching a non-zero minimum value in the limit of infinite acceleration. Similarly, it was shown that the Markov gap exhibits monotonic behavior with regard to acceleration. A function for reflected entropy was proposed which decreases monotonically with decreasing Unruh temperature for all states. (Phys. Rev. D 108 (2023) no.12, 125009)

The breakdown of effective field theory for Hawking radiation

Core member Pei-Ming Ho has formed an outstanding research group with visiting professor Hiraku Kawai, shown that in the background of a gravitational collapse, the transition amplitudes for the creation of particles for distant observers due to higher-derivative interactions grow exponentially with time. It becomes of order 1 when the collapsing matter is about a Planck length outside the horizon. As a result, the effective theory breaks down at the scrambling time, invalidating its prediction of Hawking radiation. (JHEP 01 (2022) 019). Furthermore, the time-dependence of Hawking radiation for a black hole in the Unruh vacuum, and is not robust against UV and IR effects. Furthermore, higher-derivative interactions with the background contribute to a large amplitude of particle creation that changes Hawking radiation, again invalidate the EFT approach. This unexpected large effect is related to a peculiar feature of the Hawking particle wave packets. (JHEP 03 (2023) 002)

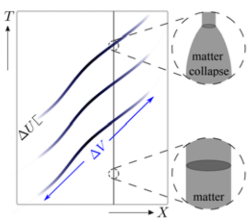


Figure 1. An outgoing wave packet with a width of ΔU can only be defined over a range of $\Delta V > 4\ell^2/\Delta U$. The vertical line represents a region considerably smaller than ΔV, consisting of matter with low density that eventually collapses into a black hole. Such a wave packet cannot be localized in the near-horizon region of the black hole, and thus will not contribute to Hawking radiation

Stringy effects on Hawking radiation and cosmological scenarios

In string theories, interactions are exponentially suppressed for trans-Planckian space-like external momenta. A study of classes of quantum field theories that exhibit this feature modeled after Witten's bosonic open string field theory reveals a Lorentz-invariant UV/IR relation that leads to the spacetime uncertainty principle proposed by Yoneya. Application to a dynamical black hole background suggests that Hawking radiation is turned off around the scrambling time. (JHEP 12 (2023) 122) The stringy space-time uncertainty relation (STUR) for inflationary cosmology was also concerned. By demanding that no fluctuation modes that exit the Hubble radius are affected by the nonlocality resulting from the STUR, we find an upper bound on the number of e-foldings of inflation. The bound is a factor of 2 weaker than what results from the Trans-Planckian Censorship Criterion (TCC). By demanding that the inflationary phase is simultaneously consistent with STUR and sufficiently long for inflation to provide a causal explanation of structure on the scale of the current Hubble radius, one finds an upper bound on the energy scale of inflation. The bound is less restrictive than what follows from the TCC, but it remains in conflict with canonical single-field inflation models. (Phys.Rev.D 109 (2024) 8, 083503)

V. (Selected) Publications (with NCTS as an affiliation only)

Chong-Sun Chu (CS):

1. J. K. Basak, A. Chakraborty, **C.S. Chu**, D. Giataganas and H. Parihar,``Massless Lifshitz field theory for arbitrary z,'' JHEP 05 (2024), 284
2. **C. S. Chu** and H. Parihar, ``Time-like entanglement entropy in AdS/BCFT,'' JHEP 06 (2023), 173
3. **C. S. Chu** and R. X. Miao, ``Chiral current induced by torsional Weyl anomaly,'' Phys. Rev. B 107 (2023) no.20, 20
4. **C. S. Chu** and A. Ito, ``Gravitational waves in metastable supersymmetry breaking,'' Phys. Rev. D 105 (2022) no.12, 123538
5. **C. S. Chu** and C. H. Leung, ``Induced Quantized Spin Current in Vacuum,'' Phys. Rev. Lett. 127 (2021) no.11, 111601
6. **C. S. Chu** and H. S. Tan, ``Generalized Darmois Israel Junction Conditions,'' Universe 8 (2022) no.5, 250

Dimitrios Giataganas (CS):

1. M. Afrasiar, J. K. Basak and **D. Giataganas**, "Timelike entanglement entropy and phase transitions in non-conformal theories," JHEP 07 (2024), 243 arXiv:2404.01393 [hep-th].
2. **D. Giataganas**, A. Kehagias and A. Riotto, "Quasinormal Modes and Universality of the Penrose Limit of Black Hole Photon Rings," JHEP, arXiv:2404.01393 [gr-qc].
3. J. K. Basak, A. Chakraborty, C. S. Chu, **D. Giataganas** and H. Parihar, "Massless Lifshitz field theory for arbitrary z," JHEP 05 (2024), 284 arXiv:2312.16284 [hep-th].
4. J. K. Basak, **D. Giataganas**, S. Mondal and W. Y. Wen, "Reflected entropy and Markov gap in noninertial frames," Phys. Rev. D 108 (2023) no.12, 125009 arXiv:2306.17490 [quant-ph].
5. **D. Giataganas**, "Velocity Laws for Bound States in Asymptotically AdS Geometries," Fortsch. Phys. 71 (2023) no.4-5, 2300030, arXiv:2301.00123 [hep-th]

Yu-tin Huang (CS):

1. Song He, Yu-tin.Huang and Chia Kai. Kuo, ``All-Loop Geometry for Four-Point Correlation Function,'' arXiv:2405.20292 (Accepted PRD Letter)
2. Katsuki. Aoki and Yu-tin. Huang, ``Anomalous Thresholds for the S-matrix of Unstable Particles,'' JHEP 09 (2024) 45
3. Li-Yuan Chiang, Yu-tin Huang, Laurentiu Rodina, and He-Chen Weng (2024, May). De-projecting the EFThedron. Journal of High

Energy Physics, JHEP 05 (2024) 102**.**
4. Li-Yuan Chiang, Yu-tin Huang, and He-Chen Weng (2024, May). Bootstrapping string theory EFT. Journal of High Energy Physics, JHEP 05 (2024) 289.
5. Li-Yuan Chiang,Zu-Chen Huang, **Yu-tin Huang**, Wei Li, Laurentiu Rodina, and He-Chen Weng (2024, Feb). The geometry of the modular bootstrap. Journal of High Energy Physics, JHEP 02 (2024) 209.
6. Song He, **Yu-tin Huang**, Chia-kai Kuo (2023, Sep). The ABJM Amplituhedron. Journal of high Energy Physics, 09 (2023) 165.
7. Song He, **Yu-tin Huang**, Chia-Kai Kuo, Zhenjie Li (2023, Feb). The two-loop eight-point amplitude in ABJM theory. Journal of High Energy Physics, JHEP02(2023)065.
8. Wei-Ming Chen, Ming-Zhi Chung, **Yu-tin Huang**, and Jung-Wook Kim (2022, Dec). Gravitational Faraday effect from on-shell amplitudes. Journal of High Energy Physics, JHEP12(2022)058.
9. Wei-Ming Chen, Ming-Zhi Chung, **Yu-tin Huang**, Jung-Wook Kim (2022, Aug). The 2PM Hamiltonian for binary Kerr to quartic in spin. Journal of High Energy Physics, JHEP08(2022)148
10. **Yu-tin Huang** and Grant N. Remmen (2022, Jul). UV-Complete Gravity Amplitudes and the Triple Product. Physical Review D, PRD 106, L021902.
11. Chi-Ming Chang, **Yu-tin Huang**, Zi-Xun Huang, Wei Li (2022, May). Bulk locality from the celestial amplitude. SciPost Physics, SciPost Phys. 12, 176 (2022).
12. William T. Emond, **Yu-Tin Huang**, Uri Kol, Nathan Moynihan, Donal O'Connell (2022, May). Amplitudes from Coulomb to Kerr-Taub-NUT. Journal of High Energy Physics, JHEP 05 (2022) 055.
13. Li-Yuan Chiang, **Yu-tin Huang**, Wei Li, Laurentiu Rodina, He-Chen Weng (2022, Mar). Into the EFThedron and UV constraints from IR consistency. Journal of High energy physics, JHEP 03 (2022) 063
14. Nima Arkani-Hamed, **Yu-tin Huang**, Jin-Yu Liu, Grant N. Remmen (2022, Mar). Causality, unitarity, and the weak gravity conjecture. Journal of High energy physics, JHEP 03 (2022) 083.
15. Nima Arkani-Hamed, Lorenz Eberhardt, **Yu-tin Huang**, Sebastian Mizera (2022, Feb). On unitarity of tree-level string amplitudes. Joournal of High Energy Physics, JHEP 02 (2022) 197.
16. **Yu-tin Huang**, Ryota Kojima, Congkao Wen, Shun-Qing Zhang (2022, Jan). The orthogonal momentum amplituhedron and ABJM amplitudes. *Journal* of High Energy Physics, JHEP 01 (2022)
17. Nima Arkani-Hamed, Tzu-Chen Huang, **Yu-tin Huang** (2021, Nov). Scattering Amplitudes For All Masses and Spins. Journal of High Energy Physics, JHEP11(2021)070
18. Bo-Ting Chen, Ming-Zhi Chung, **Yu-tin Huang**, Man Kuan Tam (2021, Oct). Minimal spin deflection of Kerr-Newman and Supersymmetric black hole. *Journal of High Energy Physics*, JHEP10(2021)011.
19. Nima Arkani-Hamed, Tzu-Chen Huang **Yu-tin Huang** (2021, May). The EFT- Hedron. *Journ*al of High Energy Physics, 05 (2021) 259.
20. **Yu-tin Huang**, Jin-Yu Liu, Laurentiu Rodina, Yihong Wang (2021, Apr). Carving out the Space of Open-String S-matrix. Journal of High Energy Physics, 04 (2021) 195.

Pei-Ming Ho (core member):
1. J. Borissova and **P. M. Ho**, ``From area metric backgrounds to the cosmological constant and corrections to the Polyakov action," Phys. Rev. D 110 (2024), 046017
2. R. Brandenberger, **P. M. Ho**, H. Kawai and W. H. Shao, ``Stringy spacetime uncertainty principle and a modified trans-Planckian censorship criterion,'' Phys. Rev. D 109 (2024), 083503
3. **P. M. Ho**, Y. Imamura, H. Kawai and W. H. Shao, ``A stringy effect on Hawking radiation,''

JHEP 12 (2023), 122

4. E. T. Akhmedov, T. L. Chau, **P. M. Ho**, H. Kawai, W. H. Shao and C.~T.~Wang, ``UV dispersive effects on Hawking radiation,'' Phys. Rev. D109 (2024), 025001
5. **P. M. Ho**, H. Kawai, H. Liao and Y. Yokokura, ``4D Weyl anomaly and diversity of the interior structure of quantum black hole,'' Eur. Phys. J. C 84 (2024) no.7, 711
6. **P. M. Ho** and H. Kawai, ``UV and IR effects on Hawking radiation,'' JHEP 03 (2023), 002
7. **P. M. Ho**, H. Kawai and Y. Yokokura, ``Planckian physics comes into play at Planckian distance from horizon,'' JHEP 01 (2022), 019

Chen-Pin Yeh (core member)

Himanshu Parihar (PD):

1. Y.~L.~Chuang and H.~Parihar, ``Change of polarization degree of light beams on propagation in curved space,'' Opt. Commun. 558 (2024), 130367
2. J.~K.~Basak, A.~Chakraborty, C.~S.~Chu, D.~Giataganas and H.~Parihar,``Massless Lifshitz field theory for arbitrary z,"JHEP \textbf{05} (2024), 284
3. J.~K.~Basak, D.~Basu, V.~Malvimat, H.~Parihar and G.~Sengupta, ``Holographic reflected entropy and islands in interface CFTs,'' JHEP 05 (2024), 143
4. C.~S.~Chu and H.~Parihar,``Time-like entanglement entropy in AdS/BCFT,"JHEP 06 (2023), 173

Thematic Group 2.3 Theoretical and Computational Astrophysics

Coordinator: Min-Kai Lin (Academia Sinica; Email: mklin@asiaa.sinica.edu.tw)

I. Brief Description

Theoretical and Computational Astrophysics (TCA) includes seven core members across northern and southern Taiwan institutions. It is managed by three Center Scientists: Min-Kai Lin (ASIAA), Hsi-Yu Schive (NTU), and Hsiang-Yi Karen Yang (NTHU). The group runs a postdoctoral fellowship program and supports research assistants. We organize academic activities and provide funding for other domestically hosted conferences. We support junior community members in attending international meetings and collaborations. In 2024, we launched a new visitor program. We have an extended affiliated members list for promoting TG opportunities and activities. In 2023—2024, TCA members published 35 articles. These include high-impact journals such as Nature Astronomy and collaborative work between group members.

The TCA's main scientific focuses are 1) Dark Matter and Cosmology, 2) Galaxy Formation and Evolution, 3) Multimessenger Astrophysics, and 4) Star and Planet Formation—these present areas of overlapping interest among Taiwanese astronomy institutes. We aim to facilitate domestic collaborations, connect the local community with the global one, and train the next generation of scientists. NCTS also provides a platform for TCA members to pool computational resources, a central component of theoretical astrophysics.

Further details can be found on the group's website: https://nctstca.github.io/.

II. Activities

- 2nd NCTS/UCAT/NTHU International Astronomy Winter School: Magnetism in Star-forming and Galactic Environments (January 31 — February 4, 2023)

This winter school was proposed by colleagues at NTHU and co-organized by NCTS. Dr. Alvina On, one of the group's postdocs, co-chaired the meeting. The conference successfully implemented diverse access arrangements, catering to participants in various time zones through on-site and online attendance, including asynchronous interaction through Slack. The hybrid format proved advantageous, drawing more interested participants than traditional on-site or online-only meetings. The poster session was engaging, promoting fruitful scientific exchange among local and international students. Additionally, the financial support provided by NCTS played a crucial role in enabling five overseas students to attend on-site. It underscores that even moderate partial support proved sufficient in incentivizing travel to Taipei, as it bolstered their case for additional funding from other sources.

Conference photo from the 2023 Winter School.

- Summer Student Programs (2023, 2024)

The group runs an 8-week Summer Student Program (SSP) annually to provide aspiring junior astronomers with hands-on research experience. Each year, the SSP admits approximately 15 students and includes international students, though the latter participates remotely. Unlike other centrally organized summer programs, the TCA SSP is unique in its decentralized approach: faculty and postdocs from across Taiwan can take on students who are dispersed to those institutions for their research projects. This is a precious resource for institutions or departments lacking a summer program, as it allows them to take on students through NCTS. The program begins with a 3-day workshop with introductory lectures given by domestic faculty and ends with a 2-day workshop for students to present their projects. These take place at different locations (e.g., NTU and NTHU). SSP students may continue to work on their projects after the program as graduate students.

For details on the 2024 program, see https://nctstca.github.io/events/202407-tcassp/.

Photos from the 2023 NCTS TCA Summer Student Program.

● Conference support

The group also supports other meetings hosted by domestic institutes. We typically fund invited speakers to these conferences. In Dec. 2023, we sponsored a Large-scale Parity Violation Workshop organized by ASIAA. In August 2024, we sponsored the 10th Galaxy Evolution Workshop at ASIAA. Notably, it was the first time that the Galaxy Workshop was held outside of Japan.

III. Visitors and International Collaborations

● Visitor Program

The group launched a joint visitor program between NCTS and ASIAA. By combining their resources, we invite world-leading figures to visit multiple institutions in Taiwan. This maximizes mutual exposure: domestic students and junior researchers can network with renowned astrophysicists and promote their work. At the same time, the visitor's positive experience and international influence raise awareness of Taiwanese astrophysics, which facilitates new collaborations and benefits future recruitment.

Our inaugural visitor was Professor Chris Reynolds from the University of Maryland (previously the Plumian Professor at the University of Cambridge), an expert on black holes, galaxies, and astroparticle physics. Professor Reynolds is also the principal investigator of the Advanced X-Ray Imaging

Satellite, a next-generation mission recently selected by NASA for funding.

● Collaborations

Professor Hsi-Yu Schive is the lead developer of the advanced GAMER Adaptive Mesh Refinement code that uses CPU and GPU to provide a versatile framework for state-of-the-art astrophysical simulations. As such, it has enabled many collaborative projects, notably between Professors Schive, Kuo-Chuan Pan, and Hsiang-Yi Yang, their students, and international collaborators from the US and Canada. Topics include active galactic nuclei, galaxy clusters, black holes, core-collapse supernovae, and dark matter.

Group postdoc Dr. Alvina On (2022—) continues to work with international researchers and former SSP students, such as those from USTH (Vietnam), Dunlap/CITA (Canada), and UCL (UK), on projects such as the impact of magnetic fields in interacting galaxies and the analysis of X-ray binaries.

IV. Highlights of Research Results

● Motivated by Professor Hsiang-Yi Yang's work on simulating the multi-wavelength properties of the Fermi and eRosita bubbles in the Milky Way Galaxy (Yang et al. 2022, Nature Astronomy), a follow-up work investigating whether tilted supermassive black hole jets could inflate symmetric bubbles was published in Tseng et al. (2024, The Astrophysical Journal) in collaboration with Professor Hsi-Yu Schive using the GAMER code.

● Core member Professor Yueh-Ning Lee presented complete, self-regulated, embedded protoplanetary disk formation models by considering all non-ideal magnetohydrodynamic effects, including ion-neutral friction, Hall effect, and Ohmic dissipation. This international collaboration, including students and researchers from France and India, showed that for a comprehensive parameter space, a universal disk size of around ten astronomical units is produced and supports recent observations of young protoplanetary disks. This work was published in The Astrophysical Journal (Lee et al., 2024).

● Group postdoc Dr. He-Feng Hsieh (2021—2023), an expert code developer, collaborated with core member Professor Kuo-Chuan Pan to extend GAMER to simulate core-collapse supernovae with a sophisticated neutrino heating and cooling treatment. They discovered a novel kilohertz gravitational wave feature from rapidly rotating core-collapse supernovae and published these results in The Astrophysical Journal (Hsieh et al., 2024).

● Group postdoc Dr. Alvina On (2022—), who specializes in cosmic magnetic fields, found that intrinsically polarized sources can easily appear unpolarized in observations. Her work cautions the community to account for this effect when analyzing the magnetic fields of galaxy clusters. Dr. On led this collaboration involving several domestic researchers and recently submitted a paper to the Publications of the Astronomical Society of Australia (On et al., 2024).

● Group postdoc Dr. Jowett Chan (NCTS postdoc, 2022—2024) worked with Professor Hsi-Yu Schive to implement novel methods for solving the Schrödinger-Poisson equations in GAMER. As a result, they successfully conducted Fuzzy Dark Matter (FDM) cosmological zoom-in simulations to investigate the tidal evolution of FDM subhalos. This work has been submitted to the Monthly Notices of the Royal Astronomical Society (Chan et al., 2024).

V. (Selected) Publications (with NCTS as an affiliation only)

A new kilohertz gravitational-wave feature from rapidly rotating core-collapse supernovae, **Hsieh, H.-F.**, Cabezon, R., Ma, L.-T., **Pan, K.-C**., 2024, ApJ, 961, 194

Can the Symmetric Fermi and eROSITA Bubbles Be Produced by Tilted Jets?
Tseng, P.-H., **Yang, H.-Y. K**., Chen, C.-Y., **Schive, H.-Y.**, Chiueh, T., 2024, ApJ, 970, 146

Dust dynamics in Hall-effected protoplanetary disks. I. Background Drift Hall Instability,
Wu, Y., **Lin, M.-K.**, Cui, C., Krapp, L., **Lee, Y.-N.**, Youdin, A.N., 2024, ApJ, 962, 173

Polar alignment of a dusty circumbinary disc – I. Dust ring formation,
Smallwood, J. L., **Lin, M.-K.**, Aly, H., Nealon, R., Longarini, C., MNRAS, 532, 1068

Protoplanetary disk size under nonideal magnetohydrodynamics: A general formalism with inclined magnetic field, **Lee, Y.-N.**, Ray, B., Marchand, P., Hennebelle, P., ApJL, 961, L28

Einstein rings modulated by wavelike dark matter from anomalies in gravitationally lensed images, Amruth, A., Broadhurst, T., Lim, J., Oguri, M., Smoot, G. F., Diego, J. M., Leung, E., Emami, R., Li, J., Chiueh, T., **Schive, H.-Y.**, Yeung, M. C. H., Li, S. K., 2023, Nature Astronomy, 7, 736

Cosmological simulations of two-component wave dark matter,
Huang, H., Schive, H.-Y., Chiueh, T., 2023, MNRAS, 522, 515

Galactic disc heating by density granulation in fuzzy dark matter simulations,
Yang, H.-Y., Chiang, B. T., Su, G.-M., Schive, H.-Y., Chiueh, T., Ostriker, J. P., 2024, MNRAS, 530, 129

Exploring the observability of surviving companions of stripped-envelope supernovae: A case study of Type Ic SN 2020oi,
Chen, H.-P., **Rau, S.-J.**, **Pan, K.-C.**, 2023, ApJ, 949, 121

AGN jet-inflated bubbles as possible origin of odd radio circles
Lin, Y.-H., **Yang, H.-Y. K.**, 2024, ApJ, 974, 269

uGMRT sub-GHz view of the Sausage cluster diffuse radio sources
Raja, R., Smirnov, O. M., Venturi, T., Rahaman, M., & **Yang, H.-Y. K.**, 2024, ApJ accepted.

Thematic Group 3.1 Computational Quantum Materials

Coordinator: Feng-Chuan Chuang (National Sun Yat-sen University; Email: fchuang@mail.nsysu.edu.tw)

I. Brief Description

Thematic Group 3.1 (TG3.1 in short) focuses on the field of "Quantum Computational Materials," with the three main research topics (1) Two-dimensional materials (2) Topological materials (3) Strongly correlated materials, which contain fascinating physics and promise high potential in technological applications. The current TG3.1 committee is comprised of seven core members, as shown below:

- Feng-Chuan Chuang (National Sun Yat-sen University)
- Yang-Hao Chan (Academia Sinica)
- Tay-Rong Chang (National Cheng Kung University)
- Guang-Yu Guo (National Taiwan University)
- Horng-Tay Jeng (National Tsing Hua University)
- Hsin Lin (Academia Sinica)
- Chi-Cheng Lee (Tamkang University)

In addition to the core members, there are about ten postdoctoral researchers, as well as thirty Ph.D. and Master's students participating in TG3.1.

II. Activities

The main activities that have been held by TG3.1 since 2023 are listed as follows:

1. 2023 NCTS-KIAS Workshop on Ab Initio Approaches to Quantum Materials, April 27-29, Taiwan
2. 2023 Summer school on First Principles Computational Materials Research-Introductory Level, June 26-27, Taiwan
3. The 21st Workshop on First-Principles Computational Materials Physics, June 29-30, 2023, Taiwan
4. 2023 Summer school on First Principles Computational Materials Research-Advance Level, August 28- September 1, Taiwan
5. NCTS Physics One-day Workshop on Many-body Effects in Quantum Materials, October 12, 2023, Taiwan
6. 2024 NCTS-KIAS Workshop on Ab Initio Approaches to Quantum Materials, April 17-19, Seoul, Korea
7. 2024 Summer school on First Principles Computational Materials Research-Introductory Level, June 24-25, Taiwan
8. 2024 Summer school on First Principles Computational Materials Research-Advance Level. August 12-16, Taiwan
9. The 22nd Workshop on First-Principles Computational Materials Physics, August 22-23, 2024, Taiwan

III. Visitors and International Collaborations

1. Prof. Robert Joynt (University of Wisconsin-Madison) visited TG3.1 in March 2023 and gave a talk at National Taiwan University for the workshop on Discrete Scale Invariance in Topological Semimetals.
2. Prof. Naoto Nagaosa (RIKEN) visited TG3.1 in June 2023 and gave a talk at National Taiwan University on Nonreciprocal transport and diode effect in superconductors. [NCTS IAC Lecture]
3. Prof. Eberhard K. U. Gross (Hebrew University) visited TG3.1 in June 2023 and gave a talk at National Taiwan University on Real-time TDDFT, the OISTR effect, and the birth of atto-magnetism. [NCTS IAC Lecture]
4. Prof. Priya Mahadevan (S. N. Bose National Centre for Basic Sciences) was invited to visit the NCTS physics division during August and

to give a talk on Why do twisted bilayers behave differently from their untwisted counterparts? at NSYSU.

5. Dr. Ching-Kai Chiu (RIKEN iTHEMS) visited TG3.1 in June 2023 and gave a talk at National Taiwan University on Searching for Moiré flat bands beyond twisted bilayer graphene.
6. Prof. Wei Ku (Tsung-Dao Lee Institute & Shanghai Jiao Tong University) was invited to visit the NCTS physics division in the end of 2023 and gave a talk at National Taiwan University on Probing a quantum Bose metal state via electrons: non-fermi liquid scattering and pseudogap.
7. Dr. Sheng-Jie Huang (Max Planck Institute for the Physics of Complex Systems, Dresden, Germany) was invited to visit NCTS physics division during December in 2023 and gave talks on Topological holography, quantum criticality, and boundary states.
8. Prof. Yi-Ting Hsu (University of Notre Dame) visited NCTS physics division in December 2023 and gave a talk on Unveiling Quasiparticle Berry Curvature Effects in the Spectroscopic Properties of a Topological Superconductor.
9. Prof. Thomas Garm Pedersen (Aalborg University, Denmark) was invited to visit NCTS physics division during two weeks. He gave a talk on Excitonic nonlinear optics at National Taiwan University.
10. Mr. Yugo Onishi (Massachusetts Institute of Technology) visited NCTS physics division in February 2024 and gave a talk on Quantum geometry, Optical property, and Energy gap.
11. Ms. Yi-Hsien Du (University of Chicago) visited NCTS physics division in February 2024 and gave a talk on Nonlinear bosonization, (Non-)Fermi liquids, and the anomalous Hall effect.
12. Mr. Tsung-Chi Wu (Department of Physics, Rutgers University) visited NCTS physics division and gave a talk on Exploring correlated topological phases in quantum materials.
13. Prof. Sergey Savrasov (Department of Physics and Astronomy, University of California, Davis, USA) was invited to visit NCTS physics division and gave a talk on Computing spin fluctuational coupling in unconventional superconductors from (almost) first principles.

IV. Highlights of Research Results

From Prof. F.C. Chuang

[1] An extensive first-principles investigation was conducted on 60 monolayer half-Heusler compounds, unveiling a family of 2D topological materials with promising electronic and stability characteristics. Six compounds, including RbBeBi, exhibit nontrivial topological insulating phases with gapless edge states, and RbBeBi may even host a charge density wave (CDW) phase. These findings lay the groundwork for novel 2D topological platforms derived from half-Heusler structures, with potential for future applications in electronics and topological devices. [Chinese Journal of Physics 86, 115-121 (2023)].

[2] The structural and topological properties of 2D pristine and Janus ilmenite oxides were explored, identifying several compounds as topological insulators and semimetals. Key materials, such as $Au_{0.5}Ag_{0.5}BiO_3$, exhibit features like van Hove singularities near the Fermi level, hinting at superconductivity and topological coexistence, alongside Rashba spin-splitting effects. These findings position 2D ilmenite oxides as promising candidates for future spintronic applications. [Chinese Journal of Physics 86, 242-254 (2023)].

[3] A comprehensive exploration of the 2D MA_2Z_4 family was conducted, revealing intriguing topological properties in five

monolayers, such as $TiSi_2Bi_4$ and $ZrGe_2As_4$. These materials exhibit nontrivial topology and stable gapless edge states, driven by spin–orbit coupling. With demonstrated thermodynamic stability, the MA_2Z_4 compounds show promising potential for applications in electronics and topological devices, encouraging future experimental studies in 2D material synthesis. [Journal of Physical Chemistry C 128, 6829-6835 (2024)].

[4] In another study exploring the 2D MA_2Z_4 family, $SrTl_2Te_4$ and $BaTl_2Te_4$ were identified as quantum spin Hall insulators with robust topological bandgaps of 97 and 28 meV, respectively. This research highlights a nontrivial topological phase driven by spin–orbit coupling and confirmed by gapless edge states and quantized spin Hall conductivity. These findings suggest that MA_2Z_4 monolayers indeed hold significant promise for spintronic applications, remaining stable under strain and electric fields, which supports their viability for future experimental and practical applications in topological materials. [Applied Physics Letters 124, 233102 (2024)].

[5] The material Y_3InC and related cubic antiperovskites were identified as potential higher-order topological insulators (HOTIs) with unique hinge states and Dirac node phases. First-principles calculations reveal a triple-point phase that, under spin–orbit coupling, transitions to a twin Dirac node structure, confirming complex topological features through Z_4 invariants. The study establishes Y_3InC as a promising candidate for experimental exploration in HOTI applications, paving the way for advanced topological device research. [New Journal of Physics 26, 073007 (2024).]

From Prof. H.T. Jeng

[6] We report the observation of a proximity-induced charge-density wave (PI-CDW) in a graphene layer interfaced with a 1T-TaS_2 substrate. Using scanning tunneling microscopy (STM) and spectroscopy (STS), combined with theoretical modeling, we demonstrate that the coexistence of a CDW and a Mott gap in 1T-TaS_2, coupled with the Dirac dispersion of electrons in graphene, enables a clear identification of the PI-CDW by ruling out alternative explanations. [Nature Communications 15, 8056 (2024).]

[7] In this study, an Sb-Bi codoped GeTe single crystal ($Ge_{0.86}Sb_{0.08}Bi_{0.06}$) that exhibits an ultrahigh figure of merit (zT) of 2.7 at 700 K, along with a record-high device zT of 1.41 over the temperature range of 300-773 K was synthesized and investigated. This exceptional zT value is attributed to the extremely low lattice thermal conductivity resulting from strong electron-phonon (EP) interactions. First-principles calculations further reveal that these remarkable EP interactions stem from Fermi surface nesting, which features a one-dimensional (double-walled) topology. [Energy & Environmental Science 17, 1904–1915 (2024).]

[8] By integrating angle-resolved photoemission spectroscopy with density functional theory, the monolayer Au-intercalated low-buckled plumbene, which is situated between the top Au Kagome layer and the bottom Pb(111) substrate was successfully resolved. Our findings reveal that the electron-phonon coupling enhances superconductivity in this unique material. [Advanced Science 10, 2300845 (2023)].

[9] Nanolamination of GaN and ZnO layers was employed through atomic layer deposition to fabricate GaN-ZnO homogeneous solid-solution thin films. Density functional theory (DFT) calculations were performed using a superlattice model for the laminated layers to evaluate the bandgaps for various atomic configurations in the solid-solution films. A significant reduction in the bandgap of the solid solutions was observed,

which was further elucidated by the DFT calculations. [Advanced Materials 35, 2207849 (2023)].

From Prof. T.R. Chang

[10] Topological semimetals with protected band crossings have garnered considerable attention in recent years. While nodal lines have been observed in some nonmagnetic materials, direct detection of gapless fourfold-degenerate antiferromagnetic (AFM) nodal lines has yet to be achieved. The discovery of an unusual gapless, fourfold-degenerate AFM Dirac nodal line in YMn_2Ge_2 is reported, based on first-principles calculations and angle-resolved photoemission spectroscopy (ARPES). [Nature Communications 15, 7052 (2024)].

[11] The Weyl equation was initially derived for odd spatial dimensions; however, extending the 3D Weyl fermion state to 2D results in a distinct topological state of matter known as a 2D Weyl semimetal, which functions as a spin-polarized analog of graphene. The realization of a 2D Weyl semimetal in an epitaxial bismuthene monolayer on SnS(Se) substrates is reported, marking the solid-state realization of Weyl fermions in 2D space. [Nature Communications 15, 6001 (2024)].

[12] Kagome magnets are provided as a fascinating platform for a plethora of topological quantum phenomena. Theoretical predictions and direct visualization of the Weyl lines in the A-A stacked kagome magnet $GdMn_6Sn_6$ are presented. Remarkably, tunable SOC gaps of the Weyl lines are observed after substituting Gd with Tb and Li, respectively. This finding paves the way for studying topological phase transitions on the Kagome lattice. [Advanced Materials 35, 2205927 (2023)].

[13] A nonlinear Hall effect induced by the quantum metric dipole is reported, achieved by interfacing even-layered $MnBi_2Te_4$ with black phosphorus. The results may enable the use of antiferromagnetic (AFM) spins to harvest electromagnetic energy and facilitate the realization of self-powered AFM spintronic devices. [Science 381, 181 (2023)].

From Prof. Y.H. Chan

[14] A Feynman diagram approach has been introduced for calculating the nonlinear optical responses of atomically thin 2D materials, emphasizing excitonic effects. It has been demonstrated that the inclusion of electron-hole interactions leads to significant qualitative changes in the second harmonic generation spectrum of monolayer h-BN compared to independent particle approximations. This method is poised to be extended to higher-order optical responses and is suitable for first-principles calculations, thereby enhancing the understanding of excitonic influences on nonlinear optical phenomena. [Physical Review B 109, 155437 (2024)].

[15] Ab initio many-body calculations using the ***G-W*** plus Bethe-Salpeter equation (***G-W-BSE***) method have been conducted to explore the exciton shift current in small-diameter zigzag BN nanotubes and a single BN sheet. It has been revealed that a significant in-gap peak in the shift current spectrum arises from the ***A*** exciton, with its peak value exceeding three times that of the quasiparticle shift current, attributed to the enhanced optical dipole matrix element. Additionally, the effective exciton shift current conductivity has been found to be nearly ten times larger than the largest shift conductivity reported in ferroelectric semiconductors, and the shift current direction was shown to be independent of tube chirality, challenging previous model predictions. [Physical Review B 108, 075413 (2023)].

[16] An ab initio many-body method has been developed to investigate nonperturbative high

harmonic generation (HHG) through the real-time propagation of the non-equilibrium Green's function with GW self-energy. Good agreement with experimental results has been achieved for monolayer MoS_2, including the characteristic patterns of monotonic and nonmonotonic harmonic yield in parallel and perpendicular responses, respectively. It has been demonstrated that many-body effects are crucial for accurately reproducing the spectral features in the perpendicular response, reflecting a complex interplay of electron-hole interactions and many-body renormalization along with the Berry curvature of the independent quasiparticle band structure. [Nature Communications 15, 6228 (2024)].

[17] Photoinduced charge transfer across atomically thin interfaces has been shown to occur within sub-50 fs time scales, despite the weak van der Waals interlayer coupling. An ab initio many-body perturbation theory approach has been employed to explicitly account for excitons and phonons in the WS_2/MoS_2 heterobilayer. Large-scale first-principles calculations reveal that the exciton–phonon interaction induces relaxation times of 67 fs and 15 fs for photoexcited excitons in the K valley of MoS_2 and WS_2 at 300 K, respectively, setting a lower bound for the intralayer-to-interlayer exciton transfer time and supporting experimental observations, while also demonstrating that electron–hole correlations enable novel transfer pathways not accessible to noninteracting charge carriers. [Nano Letters 24, 7972-7978 (2024)].

From Prof. C.C. Lee

[18] The strain dependence of angle-resolved second harmonic generation (SHG) in InSe flakes was experimentally investigated, revealing a decrease in SHG intensity with increasing compressive strain. First-principles electronic structure calculations were conducted to model strain effects on SHG susceptibilities, accurately fitting experimental data with a single fitting parameter. This approach provides a quantitative framework for understanding strain-induced SHG patterns in 2D materials, aiding the design of flexible device applications. [Nanomaterials 13, 750 (2023)].

[19] Silicon and germanium, although widely used in electronic devices, have traditionally been considered unsuitable for interconnections in integrated circuits due to their semiconducting nature. In this study, unexpected metallic monolayer structures of Si and Ge with a square lattice were discovered, demonstrating greater stability than the semimetallic silicene and germanene structures. These 2D Si and Ge allotropes were found to host Dirac fermions with Fermi velocities surpassing those of graphene, indicating that metal interconnects in silicon-based integrated circuits could be made solely from Si, allowing for fully silicon-based circuit integration. [Physical Review B 107, 115410 (2023)].

[20] The debated role of Fermi surface nesting in the charge density wave (CDW) state of 2H-$NbSe_2$ was explored. Using scanning tunneling microscopy and first-principles simulations, an energetically favorable filled phase is identified, aligning with Peierls instability and showing fully opened gaps at the CDW Brillouin zone boundary. The results reveal that Fermi surface nesting, triggered by two nesting vectors, leads to CDW formation, while a single vector results in a stripe phase. These findings position the filled phase of $NbSe_2$ as a clear example of a Peierls instability-induced CDW in 2D materials. [ACS Materials Letters 6, 2941-2947 (2024)].

From Prof. G.Y. Guo

[21] A time-reversal-even spin generation effect, occurring in the second order of electric fields, is proposed to dominate current-induced spin

polarization across a wide range of centrosymmetric nonmagnetic materials, introducing a new form of nonlinear spin-orbit torque in magnets. This effect is shown to have a quantum origin linked to the momentum space dipole of anomalous spin polarizability. First-principles calculations predict substantial spin generation in various nonmagnetic hcp metals, monolayer $TiTe_2$, and ferromagnetic monolayer $MnSe_2$, all experimentally detectable. This study significantly advances nonlinear spintronics in both magnetic and nonmagnetic systems. [Physical Review Letters 130, 166302 (2023)].

[22] Topologically protected photonic edge states enable robust photon propagation, offering potential for applications in waveguiding, lasing, and quantum information. This study reports a novel class of hybrid topological photonic crystals that exhibit both quantum anomalous Hall and valley Hall phases in distinct photonic band gaps. These hybrid topologies produce unique edge channels, where dual-band chiral and unbalanced valley Hall edge states coexist. The crystals were experimentally realized and shown to support dual-band topological edge states, which can function as frequency-multiplexing devices for beam splitting and combining. This research highlights hybrid topological insulators as a new topological phase for photons and a valuable direction in topological photonics. [Nature Communications 14, 4457 (2023)].

[23] Distinctive charge transport features originating from nontrivial bulk and surface states in topological systems present an ongoing challenge in understanding Dirac and Weyl semimetals. In this work, experimental observations reveal pronounced nonlinear and nonreciprocal transport effects in both longitudinal and transverse channels for a $SrRuO_3$ thin film on a $SrTiO_3$ substrate. The transverse nonlinear Hall signal depends on the angle α between the current direction and the orthorhombic $[001]_0$axis, reaching a peak when aligned along orthorhombic $[1\bar{1}0]_0$, while the longitudinal response is strongest along $[001]_0$ and vanishes along $[1\bar{1}0]_0$. These angle-dependent effects suggest a magnetic Weyl phase with an effective Berry curvature dipole along $[1\bar{1}0]_0$ and 1D chiral edge modes along $[001]_0$. [Physical Review X 14, 011022 (2024)].

From Prof. H. Lin

[24] In monolayer tungsten ditelluride (WTe_2), Coulomb interactions between electrons and holes can form a 2D topological excitonic insulator (2D TEI) through exciton formation. This phase uniquely combines non-trivial band topology with excitonic properties, although the precise role of Coulomb interactions in creating the 2D bulk gap of WTe_2 is still debated. Recent findings show that WTe_2 undergoes a gate-tunable quantum phase transition, where its 2D energy gap collapses upon ambipolar field-effect doping. This tunability allows WTe_2 to alternate between n- and p-type semimetals, offering control over non-trivial 2D superconductivity via excitonic pairing. [Advanced Materials 36, 2309356 (2023)].

[25] The nonlinear Hall effect (NLHE) generates a transverse Hall voltage in time-reversal-invariant materials. In $TaIrTe_4$ nanoribbons, NLHE is observed through quantum transport measurements without requiring Berry curvature dipole information. Global measurements show NLHE in both transverse directions, with quantum confinement effects seen as nanoribbon widths vary. Atomic-scale probing reveals distinct local NLHE patterns among neighboring atomic groups, linked to the non-centrosymmetric structure of $TaIrTe_4$. Optimizing probe position enables nearly an order of magnitude enhancement in Hall voltage, highlighting NLHE's potential in tunable nanoscale devices and broadening the study of

NLHE in diverse material systems. [npj Computational Materials 10, 40 (2024)].

[26] In time-reversal symmetric systems, the quantum spin Hall phase often aligns with the topological insulator phase, identified by the spin Chern number. However, monolayer α-Sb displays a unique topological phase with a spin Chern number of 2, despite being classified as trivial in standard schemes. A phase transition between α-As and α-Sb occurs via band inversions at two k points. Without spin-orbit coupling (SOC), α-As is a trivial insulator, while α-Sb forms a Dirac semimetal. SOC gaps the Dirac points, introducing a nontrivial Berry curvature in α-Sb, which shows gapless edge states, consistent with topological properties. [2D Materials 11, 025033 (2024)].

[27] Topological semimetals with protected surface states show promise for advanced electronics, improving memory, sensing, and communication. Quantum transport studies in NbAs highlight its potential for highly-scaled integrated circuits. Density functional theory (DFT) and non-equilibrium Green's function (NEGF) calculations reveal that the resistance-area (RA) product of NbAs films decreases with reduced thickness, unlike the constant RA product in ideal copper films. NbAs films maintain favorable RA scaling even with surface defects. These findings suggest that NbAs and similar topological semimetals could serve as viable materials for future back-end-of-line (BEOL) interconnects. [npj Computational Materials 10, 84 (2024)].

V. (Selected) Publications (with NCTS as an affiliation only)

[1] Aniceto B Maghirang III, Rovi Angelo B. Villaos, Zhi-Quan Huang, Chia-Hsiu Hsu, Guoqing Chang, **Feng-Chuan Chuang**, Nontrivial topological properties in two-dimensional half-Heusler compounds, Chinese Journal of Physics, 86, 115 (2023).

[2] Susaiammal Arokiasamy, Gennevieve M. Macam, Rovi Angelo B. Villaos, Aniceto B. Maghirang III, Zhi-Quan Huang, Chia-Hsiu Hsu, Guoqing Chang, and **Feng-Chuan Chuang**, Prediction of quantum spin Hall and Rashba effects in two-dimensional ilmenite oxides, Chinese Journal of Physics, 86, 242 (2023).

[3] Ina Marie R Verzola, Rovi Angelo B. Villaos, Zhi-Quan Huang, Chia-Hsiu Hsu, Yoshinori Okada, Hsin Lin, **Feng-Chuan Chuang**, Nontrivial Topology in Monolayer MA_2Z_4 (M = Ti, Zr, or Hf; A = Si or Ge; and Z = N, P, As, Sb, or Bi), Journal of Physical Chemistry C 128 (16), 6829-6835 (2024).

[4] Joel D'Souza, Ina Marie R Verzola, Sreeparvathy P.C., Rovi Angelo B. Villaos, Zhi-Quan Huang, **Feng-Chuan Chuang**, Quantum spin Hall insulating phase in two-dimensional MA_2Z_4 materials: $SrTl_2Te_4$ and $BaTl_2Te_4$, Applied Physics Letters 124 (23), 233102 (2024).

[5] Sreeparvathy PC, Rovi Angelo B. Villaos, Zhi-Quan Huang, **Feng-Chuan Chuang**, Higher-order topological Dirac phase in Y_3InC: a first-principles study, New Journal of Physics 26, 073007 (2024).

[6] Nikhil Tilak, MichaelAltvater, Sheng-Hsiung Hung, Choong-Jae Won, Guohong Li, Taha Kaleem, Sang-Wook Cheong, Chung-Hou Chung, **Horng-Tay Jeng**, & Eva Y. Andrei, Proximity induced charge density wave in a graphene/1T-TaS_2 heterostructure, Nature Communications 15, 8056 (2024).

[7] Ye-Shun Lan, Chia-Ju Chen, Shu-Hua Kuo, Yen-Hui Lin, Angus Huang, Jing-Yue Huang, Pin-Jui Hsu, Cheng-Maw Cheng, and **Horng-Tay Jeng**, Dual Dirac Nodal Line in Nearly

Freestanding Electronic Structure of β-Sn Monolayer, ACS Nano 18, 20990−20998 (2024).

[8] V. K. Ranganayakulu, Te-Hsien Wang, Cheng-Lung Chen, Angus Huang, Ma-Hsuan Ma, Chun-Min Wu, Wei-Han Tsai, Tsu-Lien Hung, Min-Nan Ou, **Horng-Tay Jeng**, Chih-Hao Lee, Kuei-Hsien Chen, Wen-Hsien Li, Madison K. Brod, G. Jeffrey Snyder and Yang-Yuan Chen, Ultrahigh zT from strong electron-phonon interactions and a low-dimensional Fermi surface, Energy and Environmental Science 17, 1904–1915 (2024).

[9] Chin-Hsuan Chen, Ye-Shun Lan, Angus Huang and **Horng-Tay Jeng**, Two-gap topological superconductor LaB_2 with high Tc = 30 K, Nanoscale Horizon. 9, 148–155 (2024).

[10] Wan-Hsin Chen, Chin-Hsuan Chen, Guan-Hao Chen, Wei-Chuan Chen, Fu-Xiang Rikudo Chen, Pei-Jung Chen, Chun-Kai Ku, Chang-Tsan Lee, Naoya Kawakami, Jia-Ying Li, Iwao Matsuda, Wen-Hao Chang, Juhn-Jong Lin, Chien-Te Wu, Chung-Yu Mou, **Horng-Tay Jeng**, Shu-Jung Tang, and Chun-Liang Lin, Enhanced Superconductivity and Rashba Effect in a Buckled Plumbene-Au Kagome Superstructure, Advanced Science 10, 2300845 (2023).

[11] Ming-Wei Liao, **Horng-Tay Jeng**, and Tsong-Pyng Perng, "Formation Mechanism and Bandgap Reduction of GaN-ZnO Solid-Solution Thin Films Fabricated by Nanolamination of Atomic Layer Deposition", Advanced Materials 35, 2207849 (2023).

[12] Ro-Ya Liu, Angus Huang, Raman Sankar, Joseph Andrew Hlevyack, Chih-Chuan Su, Shih-Chang Weng, Meng-Kai Lin, Peng Chen, Cheng-Maw Cheng, Jonathan D. Denlinger, Sung-Kwan Mo, Alexei V. Fedorov, Chia-Seng Chang, **Horng-Tay Jeng**, Tien-Ming Chuang, and Tai-Chang Chiang, Dirac Nodal Line in Hourglass Semimetal Nb_3SiTe_6, Nano Letters 23, 380−388 (2023).

[13] Xian P. Yang, Yueh-Ting Yao, Pengyu Zheng, Shuyue Guan, Huibin Zhou, Tyler A. Cochran, Che-Min Lin, Jia-Xin Yin, Xiaoting Zhou, Zi-Jia Cheng, Zhaohu Li, Tong Shi, Md Shafayat Hossain, Shengwei Chi, Ilya Belopolski, Yu-Xiao Jiang, Maksim Litskevich, Gang Xu, Zhaoming Tian, Arun Bansil, Zhiping Yin, Shuang Jia, **Tay-Rong Chang** & M. Zahid Hasan, A topological Hund nodal line antiferromagnet, Nature Communications 15, 7052 (2024).

[14] Qiangsheng Lu, P. V. Sreenivasa Reddy, Hoyeon Jeon, Alessandro R. Mazza, Matthew Brahlek, Weikang Wu, Shengyuan A. Yang, Jacob Cook, Clayton Conner, Xiaoqian Zhang, Amarnath Chakraborty, Yueh-Ting Yao, Hung-Ju Tien, Chun-Han Tseng, Po-Yuan Yang, Shang-Wei Lien, Hsin Lin, Tai-Chang Chiang, Giovanni Vignale, An-Ping Li, Tay-Rong Chang, Rob G. Moore & Guang Bian, Realization of a two-dimensional Weyl semimetal and topological Fermi strings, Nature Communications 15, 6001 (2024).

[15] Yueh-Ting Yao, Xiaoting Zhou, Yi-Chun Hung, Hsin Lin, Arun Bansil, and **Tay-Rong Chang**, Atomic Scale Quantum Anomalous Hall Effect in Monolayer Graphene/$MnBi_2Te_4$ Heterostructure, Materials Horizons 11, 3420 (2024).

[16] Yueh-Ting Yao, Xiaoting Zhou, Yi-Chun Hung, Hsin Lin, Arun Bansil, and **Tay-Rong Chang**, Feature-energy duality of topological boundary states in a multilayer quantum spin Hall insulator, Physical Review B 109, 155143 (2024).

[17] Anyuan Gao, Yu-Fei Liu, Jian-Xiang Qiu, Barun Ghosh, Thaís V. Trevisan, Yugo Onishi, Chaowei Hu, Tiema Qian, Hung-Ju Tien, Shao-Wen Chen, Mengqi Huang, Damien Bérubé,

Houchen Li Christian Tzschaschel, Thao Dinh, Zhe Sun, Sheng-Chin Ho, Shang-Wei Lien, Bahadur Singh, Kenji Watanabe, Takashi Taniguchi, David C. Bell, Hsin Lin, **Tay-Rong Chang**, Chunhui Rita Du, Arun Bansil, Liang Fu, Ni Ni, Peter P. Orth, Qiong Ma, & Su-Yang Xu, Quantum metric nonlinear Hall effect in a topological antiferromagnetic heterostructure, Science 381, 181 (2023).

[18] Jian-Xiang Qiu, Christian Tzschaschel, Junyeong Ahn, Anyuan Gao, Houchen Li, Xin-Yue Zhang, Barun Ghosh, Chaowei Hu, Yu-Xuan Wang, Yu-Fei Liu, Damien Bérubé, Thao Dinh, Zhenhao Gong, Shang-Wei Lien, Sheng-Chin Ho, Bahadur Singh, Kenji Watanabe, Takashi Taniguchi, David C. Bell, Hai-Zhou Lu, Arun Bansil, Hsin Lin, **Tay-Rong Chang**, Brian B. Zhou, Qiong Ma, Ashvin Vishwanath, Ni Ni, & Su-Yang Xu, Axion optical induction of antiferromagnetic order, Nature Materials 22, 583 (2023).

[19] Jacob Cook, Sougata Mardanya, Qiangsheng Lu, Clayton Conner, Matthew Snyder, Xiaoqian Zhang, James McMillen, Geoff Watson, **Tay-Rong Chang**, and Guang Bian, Observation of Gapped Topological Surface States and Isolated Surface Resonances in $PdTe_2$ Ultrathin Films", Nano Letters 23, 1572 (2023).

[20] Zi-Jia Cheng, Ilya Belopolski, Hung-Ju Tien, Tyler A. Cochran, Xian P. Yang, Wenlong Ma, Jia-Xin Yin, Dong Chen, Junyi Zhang, Chris Jozwiak, Aaron Bostwick, Eli Rotenberg, Guangming Cheng, Md. Shafayat Hossain, Qi Zhang, Maksim Litskevich, Yu-Xiao Jiang, Nan Yao, Niels B. M. Schroeter, Vladimir N. Strocov, Biao Lian, Claudia Felser, Guoqing Chang, Shuang Jia, **Tay-Rong Chang**, M. & Zahid Hasan, Visualization of Tunable Weyl Line in A-A Stacking Kagome Magnets, Advanced Materials 35, 2205927 (2023).

[21] Yu-Tzu Chang and **Yang-Hao Chan**, Diagrammatic approach to excitonic effects on nonlinear optical response, Physical Review B 109, 155437 (2024).

[22] Yi-Shiuan Huang, **Yang-Hao Chan**, and **Guang-Yu Guo**, Large shift currents via in-gap and charge-neutral excitons in a monolayer and nanotubes of BN, Physical Review B 108, 075413 (2023).

[23] Victor Chang Lee, Lun Yue, Mette B. Gaarde, **Yang-Hao Chan**, and Diana Y. Qiu, Many-body enhancement of high-harmonic generation in monolayer MoS_2, Nature Communications 15, 6228 (2024).

[24] **Yang-Hao Chan**, Mit H. Naik, Jonah B. Haber, Jeffrey B. Neaton, Steven G. Louie, Diana Y. Qiu, and Felipe H. da Jornada, Exciton–Phonon Coupling Induces a New Pathway for Ultrafast Intralayer-to-Interlayer Exciton Transition and Interlayer Charge Transfer in WS_2–MoS_2 Heterostructure: A First-Principles Study, Nano Letters 24, 7972–7978 (2024).

[25] Zi-Yi Li, Hao-Yu Cheng, Sheng-Hsun Kung, Hsuan-Chun Yao, Christy Roshini Paul Inbaraj, Raman Sankar, Min-Nan Ou, Yang-Fang Chen, **Chi-Cheng Lee**, and Kung-Hsuan Lin, Uniaxial Strain Dependence on Angle-Resolved Optical Second Harmonic Generation from a Few Layers of Indium Selenide, Nanomaterials 13, 750 (2023).

[26] Chin-En Hsu, Yung-Ting Lee, Chieh-Chun Wang, Chang-Yu Lin, Yukiko Yamada-Takamura, Taisuke Ozaki, and **Chi-Cheng Lee**, Atomically thin metallic Si and Ge allotropes with high Fermi velocities, Physical Review B 107, 115410 (2023).

[27] Yung-Ting Lee, Po-Tuan Chen, Zheng-Hong Li, Jyun-Yu Wu, Chia-Nung Kuo, Chin Shan Lue,

Chien-Te Wu, Chien-Cheng Kuo, Cheng-Tien Chiang, Taisuke Ozaki, Chun-Liang Lin, **Chi-Cheng Lee**, Hung-Chung Hsueh, and Ming-Chiang Chung, Revealing the Charge Density Wave Caused by Peierls Instability in Two-Dimensional $NbSe_2$, ACS Materials Letters 6, 2941-2947 (2024).

[28] Cong Xiao, Weikang Wu, Hui Wang, Yue-Xin Huang, Xiaolong Feng, Huiying Liu, **Guang-Yu Guo**, Qian Niu, and Shengyuan A. Yang, Time-Reversal-Even Nonlinear Current Induced Spin Polarization, Physical Review Letters 130, 166302 (2023).

[30] Yanan Wang, Hai-Xiao Wang, Li Liang, Weiwei Zhu, Longzhen Fan, Zhi-Kang Lin, Feifei Li, Xiao Zhang, Pi-Gang Luan, Yin Poo, Jian-Hua Jiang, and **Guang-Yu Guo**, Hybrid topological photonic crystals, Nature Communications 14, 4457 (2023).

[31] Uddipta Kar, Elisha Cho-Hao Lu, Akhilesh Kr. Singh, P. V. Sreenivasa Reddy, Youngjoon Han, Xinwei Li, Cheng-Tung Cheng, Song Yang, Chun-Yen Lin, I-Chun Cheng, Chia-Hung Hsu, David Hsieh, Wei-Cheng Lee, **Guang-Yu Guo**, and Wei-Li Lee, Nonlinear and Nonreciprocal Transport Effects in Untwinned Thin Films of Ferromagnetic Weyl Metal $SrRuO_3$, Physical Review X 14, 011022 (2024).

[32] Babu Baijnath Prasad, Guan-Fu Liu, and **Guang-Yu Guo**, Magnetism-induced second-order nonlinear optical responses in multiferroic $BiFeO_3$, Physical Review B 110, 014422 (2024).

[33] Yande Que, Yang-Hao Chan, Junxiang Jia, Anirban Das, Zhengjue Tong, Yu-Tzu Chang, Zhenhao Cui, Amit Kumar, Gagandeep Singh, Shantanu Mukherjee, **Hsin Lin**, Bent Weber, A Gate-Tunable Ambipolar Quantum Phase Transition in a Topological Excitonic Insulator, Advanced Materials 36, 2309356 (2024).

[34] Sheng Luo, Chuang-Han Hsu, Guoqing Chang, Arun Bansil, **Hsin Lin**, & Gengchiau Liang, Real space characterization of nonlinear hall effect in confined directions, npj Computational Materials 10, 40 (2024).

[35] Baokai Wang, Xiaoting Zhou, Yi-Chun Hung, Yen-Chuan Lin, **Hsin Lin**, and Arun Bansil, High spin-Chern-number insulator in α-antimonene with a hidden topological phase, 2D Materials 11, 025033 (2024).

[36] Sushant Kumar, Yi-Hsin Tu, Sheng Luo, Nicholas A. Lanzillo, Tay-Rong Chang, Gengchiau Liang, Ravishankar Sundararaman, **Hsin Lin**, & Ching-Tzu Chen, Surface-dominated conductance scaling in Weyl semimetal NbAs, npj Computational Materials 10, 84 (2024).

Thematic Group 3.2 Strongly Correlated Condensed Matter & Cold Atoms Systems

Coordinator: Chung-Hou Chung (Nat'l Yang Ming Chiao Tung Univ.; Email: chung0523@nycu.edu.tw

I. Brief Description

The members of this TG are interested in studying novel quantum many-body phenomena in solid state systems that are arising from strong electron correlations. The core members include: Stefan Kirchner (NYCU), Po-Yao Chang (NTHU), Jhih-Shih You (NTNU), Chien-Te Wu (NYCU), Shin-Ming Huang (NSYSU), Chang-Tse Hsieh (NTU). The NCTS postdocs in this TG are: Yu-Chin Tzeng and Kim Remund. The specific research topics include: 1. Topological phases of matter and Majorana fermions, 2. Novel quantum phases, quantum phase transitions in and out of equilibrium, 3 Fractionalization, quantum spin liquids, and emergent gauge theories. Our goals are: 1. Make TG's research performance along these 3 topics internationally competitive and well-recognized, 2. Establish internal collaborations within TG members and external collaborations among top institutes/researchers, 3. Foster/train young physicists. We expect to form collaboration within TG members, and comprehensively address at least one subtopic in each of the 3 main topics every year.

II. Activities

(1) The 2024 NCTS summer school：Strongly correlated physics – Numerical and Analytical approaches (Aug. 5-8, 2024). Total participants: 94, including 54 graduate students/postdocs. This summer school gathers international and domestic researchers specializing in analytical, numerical and experimental approaches to correlated phenomena. The invited speakers give tutorial lectures on (i) Dynamical mean-field theory and Numerical Renormalization Group methods, (ii) Field-theoretical Renormalization Group approach, (iii) Tensor network approach, and (iv) experimental approach (ARPES). The combined different approaches aim to give young students and postdocs an overview of the field and stimulate discussions and collaborations among them.

(2). The 2023 NCTS summer school on non-Hermitian and non- equilibrium quantum many-body systems (Aug. 31-Sep.01, 2023). Total participants: 85, including 46 graduate students. Non-Hermitian quantum physics and the dynamics of non-equilibrium systems exhibit distinct characteristics that set them apart from ordinary equilibrium quantum systems. They give rise to several surprising phenomena that have no counterparts in equilibrium settings. This summer school aims to introduce new concepts related to non-Hermitian and non-equilibrium quantum systems. Four experts delivered pedagogical lectures covering topics such as the mathematical structures underlying non-Hermitian quantum systems, the classification of non-Hermitian quantum systems, the topological aspects of non-Hermitian physics, and the dynamics of many-body quantum systems.

III. Visitors and International Collaborations

Visitors: Takashi Oka (The University of Tokyo, Japan), Ken Shiozaki (Kyoto University, Japan), Nobuyuki Okuma (Kyushu Institute of Technology, Japan), Akira Furusaki, RIKEN, Japan, Yi-Hsien Du (U. of Chicago).

International Collaborations: (i) Chung-Hou Chung and experimental group in Brookhaven National Lab (Cedomir Petrovic) "The scaled-invariant Planckian metal and quantum criticality in $Ce_{1-x}Nd_xCoIn_5$, Yung-Yeh Chang, Hechang Lei, Cedomir Petrovic*, Chung-Hou Chung*, Nature

Communications 14 (581) (2023)"; (ii) Chung-Hou Chung and experimental group at Rutgers U. (Eva Andrei) "Proximity induced charge density wave in a graphene/1T-TaS2 heterostructure, Michael A. Altvater, Seng-Hsiung Hung, Nikhil Tilak, Choong-Jae Won, Guohong Li, Sang-Wook Cheong, Chung-Hou Chung*, Hrng-Tay Jeng*, Eva Y. Anderi*, Nature Communications 15, 8056 (2024)." (iii) Chang-Tse Hsieh's group and Prof. Masaki Oshikawa of U. Tokyo "Lieb-Schultz-Mattis Theorem for 1D Quantum Magnets with Antiunitary Translation and Inversion Symmetries, Yuan Yao, Linhao Li, Masaki Oshikawa, and Chang-Tse Hsieh, Phys. Rev. Lett. 133, 136705 (2024)."

IV. Highlights of Research Results

(i). Proximity induced charge density wave in a graphene/1T-TaS2 heterostructure, Michael A. Altvater, Seng-Hsiung Hung, Nikhil Tilak, Choong-Jae Won, Guohong Li, Sang-Wook Cheong, Chung-Hou Chung*, Hrng-Tay Jeng*, Eva Y. Anderi*, Nature Communications 15, 8056 (2024).

Significance: The proximity-effect, whereby materials in contact appropriate each other's electronic-properties, is widely used to induce correlated states, such as superconductivity or magnetism, at heterostructure interfaces. To date, however, demonstrating the existence of proximity-induced charge-density-waves (PI-CDW) proves challenging. This is due to competing-effects, such as screening or co-tunneling into the parent-material, obscured its presence. Here we report the observation of a PI-CDW in a graphene layer contacted by a 1T-TaS_2 substrate. Using scanning-tunneling-microscopy (STM) and spectroscopy (STS) together with theoretical-modeling, we show that the coexistence of a CDW with a Mott-gap in 1T-TaS_2 coupled with the Dirac-dispersion of electrons in graphene, makes it possible to unambiguously demonstrate the PI-CDW by ruling out alternative interpretations. Furthermore, we find that the PI-CDW is accompanied by a reduction of the Mott gap in 1T-TaS_2 and show that the mechanism underlying the PI-CDW is well-described by short-range exchange-interactions that are distinctly different from previously observed proximity effects.

(ii). The scaled-invariant Planckian metal and quantum criticality in $Ce_{1-x}Nd_xCoIn_5$, Yung-Yeh Chang, Hechang Lei, Cedomir Petrovic*, Chung-Hou Chung*, Nature Communications 14 (581) (2023)

Significance: Perfect T-linear resistivity associated with universal scattering rate: 1/ t= a * k_B* T /(h/2p) with a ~1, so-called "Planckian metal" state, has been observed in the normal state of a variety of strongly correlated superconductors close to a quantum critical point. However, the microscopic origin of this intriguing phenomena and its link to quantum criticality still remains an outstanding open problem. In this work, we observe the quantum-critical T/B-scaling of the Planckian metal state in the resistivity and heat capacity of heavy-electron superconductor $Ce_{1-x}Nd_xCoIn_5$ in magnetic fields near the edge of anti-ferromagnetism, driven by critical Kondo hybridization at the critical doping x_c ~ 0:03. We further provide the first microscopic mechanism to account for the Planckian state in a quantum critical system based on the critical charge fluctuations near Kondo breakdown transition at xc within the quasi-two-dimensional Kondo-Heisenberg lattice model. This mechanism simultaneously captures the observed universal Planckian scattering rate as well as the quantum-critical scaling and power-law divergence in thermodynamic observables near criticality. Our mechanism is generic to Planckian metal states in a variety of quantum critical superconductors near Kondo destruction. The impacts of this paper are: (a). This is the first work to address the Planckian strange metal state both experimentally and theoretically in correlated electron systems. (b) We established research collaboration with experimentalists at Brookhaven National Lab., a world's leading laboratory in physics research. (c) Due to the similarities of strange metal states between heavy-fermions and cuprate superconductors, our results pave the way to reveal the long-standing mystery of strange metal state observed in high-Tc cuprtae superconductors since 1990s'. (d) This paper was reported in the news media and highlighted in NCTS webpage. Note: NCTS postdoc Dr. Yung-Yeh Chang is the first-author of this paper. NSTC hosted a press conference in Aug. 2023 to highlight this work.

(iii) Lieb-Schultz-Mattis Theorem for 1D Quantum Magnets with Antiunitary Translation and Inversion Symmetries, Yuan Yao, Linhao Li, Masaki Oshikawa, and Chang-Tse Hsieh, Phys. Rev. Lett. 133, 136705 (2024).

Significance: We study quantum many-body systems in the presence of an exotic antiunitary translation or inversion symmetry involving time reversal. Based on a symmetry-twisting method and spectrum robustness, we propose that a half-integer spin chain that respects any of these two antiunitary crystalline symmetries in addition to the discrete $\mathbb{Z}2\times\mathbb{Z}2$ global spin-rotation symmetry must either be gapless or possess degenerate ground states. This explains the gaplessness of a class of chiral spin models not indicated by the Lieb-Schultz-Mattis theorem and its known extensions. Moreover, we present symmetry classes with minimal sets of generators that give nontrivial Lieb-Schultz-Mattis-type constraints, argued by the bulk-boundary correspondence in 2D symmetry-protected topological phases as well as lattice homotopy. Our results for detecting the ingappability of 1D quantum magnets from the interplay between spin-rotation symmetries and magnetic space groups are applicable to systems with a broader class of spin interactions, including Dzyaloshinskii-Moriya and triple-product interactions.

(iv) General properties of fidelity in non-Hermitian quantum systems with PT symmetry Yi-Ting Tu, Iksu Jang, Po-Yao Chang, and Yu-Chin Tzeng, Quantum 7, 960 (2023)

Significance: The fidelity susceptibility is a tool for studying quantum phase transitions in the Hermitian condensed matter systems. Recently, it has been generalized with the biorthogonal basis for the non-Hermitian quantum systems. From the general perturbation description with the constraint of parity-time (PT) symmetry, we show that the fidelity F is always real for the PT-unbroken states. For the PT-broken states, the real part of the fidelity susceptibility Re[XF] is corresponding to considering both the PT partner states, and the negative infinity is explored by the perturbation theory when the parameter approaches the exceptional point (EP). Moreover, at the second-order EP, we prove that the real part of the fidelity between PT-unbroken and PT-broken states is ReF=1/2. Based on these general properties, we study the two-legged non-Hermitian Su-Schrieffer-Heeger (SSH) model and the non-Hermitian XXZ spin chain. We find that for both interacting and non-interacting systems, the real part of fidelity susceptibility density goes to negative infinity when the parameter approaches the EP, and verifies it is a second-order EP by ReF=1/2

V. (Selected) Publications (with NCTS as an affiliation only)

2023

[1] Yung-Yeh Chang, Hechang Lei, Cedomir Petrovic*, Chung-Hou Chung*, The scaled-invariant Planckian metal and quantum criticality in Ce1-xNdxCoIn5, Nature Communications 14 (581) (2023).

[2] Yu-Chin Tzeng, Po-Yao Chang, Min-Fong Yang, Interaction-induced Metal to Topological

Insulator transition, Phys. Rev. B 107, 155106 (2023).
[3] Yi-Ting Tu, Iksu Jang, Po-Yao Chang, and Yu-Chin Tzeng, General properties of fidelity in non-Hermitian quantum systems with PT symmetry, Quantum 7, 960 (2023).
[4] Yi-Cheng Wang, Hsiang-Hau Jen, Jhih-Shih You, Scaling laws for non-Hermitian skin effect with long-range couplings Phys. Rev. B 108, 085418(2023).
[5] Hsiu-Chuan Hsu, Jhih-Shih You, Junyeong Ahn, Guang-Yu Guo, Nonlinear photoconductivities and quantum geometry of chiral multifold fermions, Phys. Rev. B 107, 155434 (2023).
[6] Wei-Chi Chiu, Guoqing Chang, Gennevieve Macam, Ilya Belopolski, Shin-Ming Huang, Robert Markiewicz, Jia-Xin Yin, Zi-Jia Cheng, Chi-Cheng Lee, Tay-Rong Chang, Feng-Chuan Chuang, Su-Yang Xu, Hsin Lin, M. Zahid Hasan & Arun Bansil, Causal structure of interacting Weyl fermions in condensed matter systems, Nature Comm. 14, 2228 (2023).
[7] M. R. Lin, W. J. Li and S. M. Huang, Quaternion-based machine learning on topological quantum systems, Mach. learn.: sci. technol. 4, 015032 (2023).
[8] Bikash Patra, Rahul Verma, Shin-Ming Huang, Bahadur Singh, Role of effective mass anisotropy in realizing a hybrid nodal-line fermion state, Phys. Rev. B 108, 235136 (2023),
[9] Yi-Cheng Wang, Kuldeep Suthar, H. H. Jen, Yi-Ting Hsu and Jhih-Shih You, Non-Hermitian skin effects on thermal and many-body localized phases, Phys. Rev. B 107, L220205 (2023).

2024

[1] Iksu Jang, Po-Yao Chang, Prethermalization and transient dynamics of the Multi-Channel Kondo systems under generic quantum quench: Insights from Large-N Schwinger-Keldysh approach, Phys. Rev. B 109, 144305 (2024).
[2] Chih-Yu Lo, Po-Yao Chang, Topological entanglement entropy for torus-knot bipartitions and the Verlinde-like formulas, J. High Energy. Phys. 02, 117 (2024).
[3] Boundary conditions and anomalies of conformal field theories in 1+1 dimensions, Linhao Li, Chang-Tse Hsieh, Yuan Yao, Masaki Oshikawa, Phys. Rev. B 110, 045118 (2024).
[4] Nguyen Nhat Quyen, Wen-Yen Tzeng, Chih-En Hsu, I-An Lin, Wan-Hsin Chen, Hao-Hsiang Jia, Sheng-Chiao Wang, Cheng-En Liu, Yu-Sheng Chen, Wei-Liang Chen, Ta-Lei Chou, I-Ta Wang, Chia-Nung Kuo, Chun-Liang Lin, Chien-Te Wu, Ping-Hui Lin, Shih-Chang Weng, Cheng-Maw Cheng, Chang-Yang Kuo, Chien-Ming Tu, Ming-Wen Chu, Yu-Ming Chang, Chin Shan Lue, Hung-Chung Hsueh and Chih-Wei Luo, Three-dimensional ultrafast charge-density-wave dynamics in CuTe, Nature Communication 15, 2386 (2024).
[5] Yung-Ting Lee, Po-Tuan Chen, Zheng-Hong Li, Jyun-Yu Wu, Chia-Nung Kuo, Chin-Shan Lue, Chien-Te Wu, Chien-Cheng Kuo, Cheng-Tien Chiang, Chun-Liang Lin, Chi-Cheng Lee, Hung-Chung Hsueh, Ming-Chiang Chung, Revealing the Charge Density Wave Caused by Peierls Instability in Two-Dimensional NbSe, ACS Materials Letter 6, 2941 (2024).
[6] Bastian Noßmann, Zuodong Yu, Ankur Das, Stefan Schulte, Nicolas Néel, Chien-Te Wu, Stefan Kirchner, Jörg Kröger,”Yu–Shiba–Rusinov states induced by single Fe atoms on reconstructed compound superconductor V3Si, Surface Science 746, 122504 (2024).
[7] Yuan Yao, Linhao Li, Masaki Oshikawa, Chang-Tse Hsieh, Lieb-Schultz-Mattis theorem for 1d quantum magnets with antiunitary translation and inversion symmetries, Phys. Rev. Lett. 133, 136705 (2024).
[8] Jiunn-Wei Chen, Chang-Tse Hsieh, Ryutaro Matsudo, Boundary condition and reflection anomaly in 2+1 dimensions, SciPost Physics 17 (2), 068(2024).
[9] R.-Z. Lin, H. Jin, P. Klavins, W.-T. Chen, Y.-Y. Chang, C.-H. Chung, V. Taufour, and C.-L.

Huang, Non-Fermi-liquid behavior consistent with a preasymptotic disorder-tuned ferromagnetic quantum critical point in the heavy fermion system CeTi1−xVxGe3, *Phys. Rev. Research* 6, 033130 (2024).
[10] Yung-Yeh Chang, Khoe Van Nguyen, Kuang-Lung Chen, Yen-Wen Lu, Chung-Yu Mou, and Chung-Hou Chung*, Correlation-driven Topological Kondo superconductors, Communications Physics 7, 253 (2024).
[11] Nikhil Tilak, Michael Altvater, Sheng-Hsiung Hung, Choong-Jae Won, Guohong Li, Taha Kaleem, Sang-Wook Cheong, Chung-Hou Chung*, Horng-Tay Jeng*, and Eva Andrei*, Proximity Induced Charge Density Wave in a Graphene 1T/TaS_2 Heterostructure, Nature Communications 15, 8056 (2024).
[12] Jiunn-Wei Chen, Chang-Tse Hsieh, Ryutaro Matsudo, Boundary condition and reflection anomaly in 2 + 1 dimensions, SciPost Phys. 17, 068 (2024).

Thematic Group 4.1 High-Performance Computing and Machine Learning

Coordinator: Pochung Chen (National Tsing Hua University; Email: pcchen@phys.nthu.edu.tw)

I. Brief Description

In this thematic group, we leverage high-performance computing and machine learning to explore strongly correlated many-body systems. Our focus is on understanding quantum entanglement and topological order, both in and out of equilibrium. The group is coordinated by Prof. Pochung Chen (CS, NTHU), with core members including Prof. Chia-Min Chung (CS, NSYSU), Prof. Yi-Ping Huang (CS, NTHU), Prof. Ming-Chiang Chung (NCHU), Prof. Hsiu-Chuan Hsu (NCCU), Prof. Ching-Yu Huang (THU), and Prof. Yu-Cheng Lin (NCCU). Together, we're advancing research in this exciting area of quantum systems.

II. Activities

We host international online seminar series to stay connected with global communities and leading experts, fostering opportunities for new collaborations. Our workshops are designed to strengthen internal connections and engage a broader audience interested in collaborative research. Additionally, we organize educational schools to introduce students and early-career scientists to essential concepts and techniques in this field. Here are some of our recent activities:

CompQu Seminar Series

We host the "Computational Quantum Material (CompQu)" seminar series, where leading experts share their latest breakthroughs at the forefront of the field. So far, we've organized 14 talks spanning 2023-2024, each bringing fresh insights and advancements to our community.

Workshops

- (March. 24~29, 2024) We co-organized an international workshop with SQAI program in Japan, "SQAI-NCTS Workshop on Tensor Network and Quantum Embedding"

In collaboration with the SQAI program, we co-organized the *SQAI-NCTS Workshop on Tensor Network and Quantum Embedding*, an international conference bringing together Taiwan's National Center for Theoretical Sciences (NCTS) and Japan's Sustainable Quantum AI (SQAI) project. The event highlighted quantum-inspired algorithms and their expanding applications, with speakers joining from Japan, the United States, France, China, and Taiwan.

The conference explored topics including many-body physics, quantum computing, statistical mechanics, and advanced algorithms built on tensor networks. One of the exciting emerging areas discussed was the use of tensor networks as data structures for optimizing high-dimensional integration and function representation—an approach that is advancing rapidly thanks to global research efforts and holds great promise for future breakthroughs.

- (July. 31~Aug. 1, 2024) **We organize a mini-workshop: Advanced tensor network applications.**

This mini-workshop focuses on the new frontier of quantics tensor train and novel tensor network algorithms. We invited speakers from Europe and Japan to deliver advanced research talks.

- (Jan. 22~Jan. 23, 2024) **We organize a mini-workshop: Tensor Network algorithms and applications.**

This mini-workshop focuses on the frontier of correlated physics and machine learning with tensor network algorithms. We invited speakers from Japan, Korea, and Europe to deliver frontier research talks.

- (June. 7~9, 2023) **We co-organized the cross-TG workshop, "The Future is non-perturbative", focused on synergy between high-energy physics and strongly correlated physics.**

This is the third installment of the Workshop series "The Future is ...". In this edition, we will discuss non-perturbative phenomena at the cross-section of QCD, condensed matter, and beyond standard model physics. We aim to bridge the gap and to initiate the dialogue between experts in these key areas to understand better the role of non-perturbative inputs, as well as future opportunities, for new physics searches. We invited speakers from Europe and the United States to deliver cutting-edge research talks.

Schools

- (Aug. 5~8, 2024) **We co-organized the cross-TG Summer School, "2024 Strongly Correlated Physics – Numerical and Analytical Approaches", focused on cutting-edge methods in strongly correlated physics.**

Strongly correlated systems are a rich resource for theoretical physics, fueling insights across high-energy physics, complex systems, and computational science. For example, superconductors shed light on spontaneous symmetry breaking in gauge theories, spin glasses reveal scale-emergent phenomena, and tensor networks have valuable applications in quantum computing.

To delve into the essentials of strongly correlated physics, we teamed up with research groups TG3.2 and TG4.1, alongside key experimental scientists. Using the renormalization group as a foundation, we connected numerical, theoretical, and experimental perspectives. We invited speakers from Japan, Germany, the United States, Canada, and Vietnam to deliver courses aimed at inspiring young researchers. The school covered numerical techniques, theoretical models, measurement approaches, and field theory, along with hands-on tutorials to provide students with practical experience in theory development and implementation. There are more than 30 participants.

- (Aug. 28~30, 2023) **We organized the Summer School, "2023 Tensor Network and Quantum Computing for Strongly Correlated Systems", focused on cutting-edge methods in strongly correlated physics.**

Quantum entanglement serves as a fundamental distinction between quantum many-body systems and single-body systems. The inherent complexity of many-body wave functions poses significant challenges in efficiently characterizing, calculating, and predicting the behavior of these systems, which is essential for advancing our research and applications in quantum many-body physics. To address this, tensor networks have emerged as a framework for describing the entanglement structure of many-body wave functions, allowing for the capture of subtle correlations.

This summer school focuses on the applications of tensor networks in many-body physics, offering a concise yet systematic curriculum for interested undergraduate and graduate students. The program includes practical exercises and features expert lectures from prominent researchers in the field, emphasizing both fundamental theory and hands-on skills. We invited speakers from Europe, Australia, and the United States to deliver courses aimed at inspiring young researchers. There are more than 30 participants.

III. Visitors and International Collaborations

In the past two years, we have invited international visitors and collaborated with the following international researchers. Through their visits, we aim to strengthen international collaborations with domestic researchers.

- Prof. Chisa Hotta (University of Tokyo, Japan)
- Prof. Xavier Waintal (SUNY Stony Brook, USA)
- Prof. Ching-Kai Chiu (RIKEN, Japan)
- Prof. Hsing-Ta Chen (University of Notre Dame, USA)
- Prof. Shiwei Zhang (Flatiron Institute, USA)
- Prof. Steven R. White (University of California, Irvine, USA)
- Prof. Ulrich Schollwöck (LMU München, Germany)
- Prof. Michele Burrello (University of Copenhagen, Denmark

IV. Highlights of Research Results

In Science (2024) [Science 384, eadh7691 (2024)], Prof. Chia-Min Chung and collaborators examine superconductivity in the two-dimensional Hubbard model with a focus on high-temperature superconductors. Using computational methods like density matrix renormalization group (DMRG) and auxiliary-field quantum Monte Carlo (AFQMC), the research finds superconductivity in both electron- and hole-doped regions, with stronger effects on the hole-doped side where it coexists with stripe and spin-density wave (SDW) patterns. These stripes are "partially filled," with their structure and stripe filling changing based on system size and conditions. Similar patterns have been seen in high-Tc materials. This study highlights the Hubbard model's role in exploring the mechanisms behind high-Tc superconductivity and provides valuable insights into electron interactions in doped systems.

In [Phys. Rev. Res. 5, 043249 (2023)], Prof. Yu-Cheng Lin and Pochung Chen with collaborators investigate how randomness and permutation symmetry affect the quantum states in a disordered spin-2 Heisenberg chain. Using a technique called tensor network renormalization, the authors explore how spin interactions vary under different levels of randomness and bond alternation. They find that in highly disordered chains, random singlet phases emerge where spin pairs form long-distance, disordered bonds, similar to the behavior seen in lower spin systems. The study also shows how topological order and unique phases like the Haldane phase persist even when randomness is added, which has implications for understanding disorder in quantum materials. This work provides a detailed analysis of how disorder and symmetry influence quantum spin chains, contributing to the broader understanding of phase transitions and order in disordered quantum systems.

In [Phys. Rev. B 107, 205123 (2023)], Prof. Ching-Yu Huang, Pochung Chen, and collaborators developed a new method for studying phase transitions in the two-dimensional Ising model using tensor network techniques. They applied finite-size scaling, a method that allows researchers to analyze critical points in systems of limited size, by leveraging tensor networks to simplify complex calculations in the Ising model. By using a higher-order tensor renormalization group (HOTRG), they accurately determined critical properties like temperature and critical exponents with minimal error. This study shows that increasing the bond dimension in their method further refines accuracy, demonstrating the potential of tensor networks to explore phase transitions in other complex models as well.

In [Phys. Rev. B 107, 214451 (2023)], Ming-Chiang Chung and collaborators used deep learning to study phase transitions in quantum spin chains by analyzing correlation functions.

The team employed convolutional neural networks to detect different quantum phases without prior information, using spin-spin correlations as input data. This machine learning approach successfully identified phase boundaries and captured distinct phases, showing that neural networks can serve as powerful tools for recognizing complex quantum states and understanding phase transitions in quantum materials, particularly in unsupervised learning setups.

V. (Selected) Publications (with NCTS as an affiliation only)

2024

- H. Xu, **Chia-Min Chung**, M. Qin, U. Schollwöck, S. R. White, and S. Zhang, *Coexistence of Superconductivity with Partially Filled Stripes in the Hubbard Model*, Science **384**, eadh7691 (2024).
- M. M. Wauters, **Chia-Min Chung**, L. Maffi, and M. Burrello, *Simulations of the Dynamics of Quantum Impurity Problems with Matrix Product States*, Phys. Rev. B **109**, 115101 (2024).
- Yung-Ting Lee, Po-Tuan Chen, Zheng-Hong Li, Jyun-Yu Wu, Chia-Nung Kuo, Chin-Shan Lue, Chien-Te Wu, Chien-Cheng Kuo, Cheng-Tien Chiang, Chun-Liang Lin, Chi-Cheng Lee, Hung-Chung Hsueh, **Ming-Chiang Chung**., *Revealing the Charge Density Wave Caused by Peierls Instability in Two-Dimensional NbSe2*, ACS Mater. Lett. **6**, 2941 (2024).

2023

- Y.-T. Lin, S.-F. Liu, **Pochung Chen**, and **Yu-Cheng Lin**, *Random Singlets and Permutation Symmetry in the Disordered Spin-2 Heisenberg Chain: A Tensor Network Renormalization Group Study*, Phys. Rev. Res. **5**, 043249 (2023). **合作論文**
- **Ching-Yu Huang**, Sing-Hong Chan, Ying-Jer Kao, and **Pochung Chen**, Tensor network based finite-size scaling for two-dimensional Ising model, Phys. Rev. B 107, 205123 (2023) **合作論文**
- **Ming-Chiang Chung**, Guang-Yu Huang, Ian P. McCulloch, and Yuan-Hong Tsai, Deep learning of phase transitions for quantum spin chains from correlation aspects, Phys. Rev. B 107, 214451 (2023)
- M. M. Wauters, **Chia-Min Chung**, L. Maffi, and M. Burrello, *Topological Kondo Model out of Equilibrium*, Phys. Rev. B **108**, L220302 (2023).

Thematic Group 4.2 Nanoscale Physics and Chemistry

Coordinator: Liang-Yan Hsu (National Taiwan University; Email: lyhsu@gate.sinica.edu.tw)

I. Brief Description

With the great advancement of nanotechnology, the physical and chemical properties of molecules at the nanoscale have attracted considerable attention due to their emergent novel phenomena and promising application prospects. To properly describe these emergent novel phenomena, molecular simulation becomes an indispensable ingredient in nanoscale physics and chemistry. Traditionally, the computational simulations for electrons in small molecules and molecular dynamics at various levels of coarse-graining can be routinely solved for standard problems with reasonable precision. However, at the nanoscale, the state-of-art computational approaches cannot properly describe these emergent novel phenomena due to the inherent limitations of conventional theories. As a consequence, it is important to develop new theories related to molecular simulation and computational methodologies to better understand these emergent phenomena in nanoscale physics and chemistry.

Considering the strengths and opportunities for Taiwan in nanoscale physics and chemistry, our thematic group lays out three important areas:

I. Polariton chemistry and QED chemistry

II. Catalysis at the nanoscale

III. Machine learning in nanoscale physics and chemistry

The thematic group is organized by the two center scientists: Liang-Yan Hsu (AS) and Chao-Ping Hsu (AS), and five core members: Michitoshi Hayashi (NTU), Chun-Wei Pao (AS), Ming-Kang Tsai (NTNU), Cheng-Chau Chiu (NSYSU), and Min-Yeh Tsai (CCU).

II. Activities

To improve the interactions in the community, during the past two years, we hold several workshops as follows,

(1)Workshop: Plasmon, Polariton, and Quantum Electrodynamics in Physical Chemistry (Feb 6th, 2023)

We invited Prof. George Schatz, a member of the National Academy of Sciences, USA), to give a plenary talk. Many participants joined the workshop and their backgrounds ranged from chemistry, physics, and photonics. We achieved the original goal of this workshop. The workshop includes a plenary talk, research talks, and tutorial talks. It can cover people with different levels and backgrounds. We believe that this activity can improve the interactions among different fields in Taiwan.

(2) NCTS-KIAS Workshop (Apr 27th – 29th, 2023)

This workshop was co-organized by NCTS and KIAS, focusing on computational condensed matter physics. The first-year workshop was hold in Taipei, Taiwan. The activity improves the collaboration between TG3.1 and TG4.2. I believe that it will be very helpful if people in computational chemistry and physical chemistry can understand the methods developed by computational physics.

(3) ICMS 2023:

The international conference ICMS 2023 was co-organized by many core members of TG 4.2 (Prof. Cheng-Chau Chiu, Prof. Michitoshi Hayashi, Prof. Ming-Kang Tsai). This conference is the first large-scale, international conference on theoretical and computational chemistry/molecular simulation conference to be held in Taiwan after the COVID-19 epidemic. There are about 300 participants from 21 countries, including two academicians of the National Academy of Sciences, Michael Klein and William A Goddard III (Member of the National Academy of Sciences, USA). On the one hand, this conference demonstrates the amount of domestic research in theoretical and computational chemistry Able to achieve common ground and diversity, while also promoting exchanges and cooperation between domestic scholars and foreign countries.

(4) KIAS-NCTS Workshop (Apr 17th -19th, 2024)
The second-year workshop was hold in Seoul, South Korea. The activity improves the collaboration between TG3.1, TG4.2, and computational condensed physics in Korea.

(5) Frontier Topics in Physics, Chemistry & Biology 2024 (Sept 20th -21th, 2024)
To provide domestic scholars engaged in interdisciplinary related research with the opportunity to exchange research experiences with each other and enhance exchanges between various research groups (including physics, chemistry, and biology), TG4.2 and TG4.3 jointly organized this interdisciplinary seminar meeting. Speakers are active members from TG4.2 (Nanoscale Physics and Chemistry) and TG4.3 (Complex Systems) who present their research expertise to promote the exchange of ideas and possible collaboration on topics of common interest and provide sufficient time for discussion. Scholars, students, and postdoctoral researchers studying in related fields are welcome to register. The conference can enhance and promote research cooperation in related interdisciplinary research fields in Taiwan.

III. Visitors and International Collaborations

In 2023, we invited Prof. George Schatz (Northwestern University), Prof. Seogjoo Jang (City University of New York), Prof. Henryk Witek (NYCU), Prof. Chern Chuang (University of Nevada), Dr. Andrei Gasic (Rice University), Prof. Akbar Salam (Wake Forest University), Prof. Yu-Shan Lin (Tufts University), and Prof. Shannon Yan (Stanford University) to give seminar talks in order to improve international collaboration.

In 2024, we invited Prof. Hsing-Ta Chen (University of Notre Dame), Dr. Jheng-Wei Li (CEA Centre de Grenoble), and Prof. Ka Un Lao (Virginia Commonwealth University) to give seminar talks and share their research ideas.

The seminars were held by NCTS and T2ComSA (Taiwan Theoretical and Computational Molecular Sciences Association). I believe that these activities improve the interaction between the National Center for Theoretical Sciences and the community in computational chemistry

IV. Highlights of Research Results

(1) Polaritonic Huang-Rhys factor [J. Phys. Chem. Lett., 14, 2395-2401, (2023)): Quantifying light-matter interactions in media is a key issue in polariton chemistry and QED chemistry. Motivated by the traditional Huang-Rhys factor in chemical physics and condensed matter physics, Prof. Liang-Yan Hsu (AS) established a series of concepts, including the polaritonic Huang-Rhys factor and reorganization dipole self-coupling. Their magnitudes given by the study are in good agreement with previous experimental results. We believe that this study will provide a useful perspective on quantifying light-matter interactions in media because the traditional Huang-Rhys factor has been extensively employed to describe vibronic coupling in molecules and solids.

(2) Quantum Electrodynamic Internal Conversion Theory [J. Phys. Chem. Lett., 14,

5924-5931 (2023)]: A non-adiabatic effect is a fundamental topic in physics and chemistry, and it is very common in realistic physical chemistry systems. In QED chemistry, most studies are based on the Born-Oppenheimer approximation and do not consider the non-adiabatic effect. Prof. Liang-Yan Hsu (AS) extended the concept of the Born-Huang expansion and generalized classical theories developed by S. H. Lin and J. Jortner in the framework of traditional quantum electrodynamics. We believe that the study will enhance the academic interactions between physics and chemistry in Taiwan.

(3) Quantum Electrodynamic Electron Transfer Theory [J. Phys. Chem. Lett., 15, 7403-7410 (2024)]: Electron transfer is one of the most important and common reactions in chemistry. Prof. Liang-Yan Hsu (AS) generalized the famous Marcus theory (1992 Nobel Prize in Chemistry) to include the radiative electron transfer process and developed a unified theory of electron transfer in the framework of macroscopic quantum electrodynamics. We found that the theory shows that quantum electrodynamic effects can significantly enhance the kinetic rate of electron transfer by several orders of magnitude, and the proposed mechanism is supported by experimental reports. We believe that opening up the exploration of cavity-free quantum electrodynamic chemical reactions.

(4) Anomalous Superradiance by Polariton [Phys. Rev. Lett. 133, 128001 (2024)]: To properly describe the collective effects in QED chemistry, we developed a new formalism based on macroscopic quantum electrodynamics. Based on our studies, we found that, in the weak coupling regime, the lack of counter-rotating interactions results in the absence of the Casimir-Polder potentials (medium-assisted energy shifts) in the ground-state molecules and a significant deviation of the intermolecular dipole-dipole interactions. Furthermore, we found that the intermolecular dipole-dipole interaction cannot be neglected in QED chemistry. Moreover, we applied formalism to study superradiance in molecular aggregates coupled to polaritons. After 70 years of Dicke's seminal work, we unveiled a new type of superradiance in molecular aggregates coupled to surface plasmon polaritons, and its emission rate distinguishably surpasses the well-known Dick's N scaling law. I believe that this work has a huge impact on AMO physics in Taiwan and international societies.

(5) Spectral Density in Charge Transport [J. Chem. Theory Conptut., 20, 6981-6991 (2024); J. Chem. Phys., 159, 034103 (2023)]: Prof. Chao-Ping Hsu (AS) explored the spectral density functions for both diagonal and off-diagonal disorder in the charge transporting systems. The low-frequency region of off-diagonal disorder was clearly characterized for the first time, thanks to previously developed machine learning models, which allows fast and greedy ensemble and long-time correlation functions can be calculated. The team has also shown that the outer-shell reorganization energy for charge transport in nonpolar system can be significant. A related perspective article was also published, discussing ion the generalization of Marcus theory to two-state photophysical processes.

(6) Excited-State Charge Transfer Coupling [Phys. Chem. Lett. 14, 6126 (2024)]: Prof. Chao-Ping Hsu (AS) collaborated with Prof. Weitao Yang (Duke University, USA) and found that quasi-particle energy can offer a good description on excited-state charge-transfer coupling.

V. (Selected) Publications (with NCTS as an affiliation only)

1. Wei, Y.-C.; Hsu, L.-Y.* Polaritonic Huang–Rhys Factor: Basic Concepts and Quantifying Light–Matter Interactions in Media, J. Phys.

Chem. Lett., 14, 2395-2401 (2023).
2. Lee, M.-W.; Hsu, L.-Y.* Polariton-Assisted Resonance Energy Transfer beyond Resonant Dipole-Dipole Interaction: A Transition-Current-Density Approach, Phys. Rev. A, 107, 053709 (2023).
3. Tsai, H.-S.; Shen, C.-E.; Hsu, S.-H.; Hsu, L.-Y.* Effects of Non-Adiabatic Electromagnetic Vacuum Fluctuations on Internal Conversion, J. Phys. Chem. Lett., 14, 5924-5931 (2023).
4. Hang, C.-C.; Hsu, L.-Y.* Many-Body Coherence in Quantum Transport, Phys. Rev. B, 108, 125422 (2023).
5. Wang, Y.-S.; Wang, C.-I. Yang, C.-H.; Hsu, C.-P.* Machine-Learned Dynamic Disorder of Electron Transfer Coupling. J. Chem. Phys., 159, 034103 (2023).
6. Hsu, S.-B.; Hsu, C.-P.* On the Three Dimensional Competition Systems Arising from Arabidopsis Clock. Discrete and Continuous Dynamical Systems - B, 28, 3925–3954 (2023).
7. Chang, Y.-W.* Continuum Model Study of Optical Absorption by Hybridized Moire Excitons in Transition Metal Dichalcogenide, Phys. Rev. B, 108, 155424 (2023).
8. Hong, L.-H.; Feng, W.-J.; Chen, W.-C.; Chang, Y.-C. Highly Efficient and Well-defined Phosphinous Acid-ligated Pd(ii) Precatalysts for Hirao Cross-coupling Reaction, Dalton Trans., 52, 5101–5109 (2023).
9. Chuang, Y.-T.; Hsu, L.-Y.*; Quantum Dynamics of Molecular Ensembles Coupled with Quantum Light: Counter-rotating Interactions as an Essential Component, Phys. Rev. A, 109, 013717 (2024).
10. Chuang, Y.-T.; Hsu, L.-Y.*; Microscopic Theory of Exciton–Polariton Model Involving Multiple Molecules: Macroscopic Quantum Electrodynamics Formulation and Essence of Direct Intermolecular Interactions, J. Chem. Phys., 160, 114105 (2024).
11. Tsai, H.-S.; Shen, C.-E.; Hsu, L.-Y.*; Generalized Born–Huang Expansion under Macroscopic Quantum Electrodynamics Framework, J. Chem. Phys., 160, 144112 (2024).
12. Wei, Y.-C.*; Hsu, L.-Y.*; Wide-Dynamic-Range Control of Quantum-Electrodynamic Electron Transfer Reactions in the Weak Coupling Regime, J. Phys. Chem. Lett., 15, 7403-7410 (2024).
13. Chuang, Y.-T.; Hsu, L.-Y.*; Anomalous Giant Superradiance in Molecular Aggregates Coupled to Polaritons, Phys. Rev. Lett., 133, 128001 (2024).
14. Yang, C.-H.; Wang, C.-I.; Wang, Y.-S.; Hsu, C.-P.* Non-Negligible Outer-Shell Reorganization Energy for Charge Transfer in Nonpolar Systems. J. Chem. Theory Comput. 20, 6981–6991 (2024).
15. Lin, H.-H.; Wang, C.-I.; Yang, C.-H.; Secario, M. K.; Hsu, C.-P.* Two-Step Machine Learning Approach for Charge-Transfer Coupling with Structurally Diverse Data. J. Phys. Chem. A 128, 271–280 (2024).
16. Kuan, K.-Y.; Yeh, S.-H.; Yang, W.; Hsu, C.-P.* Excited-State Charge Transfer Coupling from Quasiparticle Energy Density Functional Theory. J. Phys. Chem. Lett., 15, 6126–6136 (2024).
17. Kuan, K.-Y.; Hsu, C.-P.* Predicting Selectivity with a Bifurcating Surface: Inaccurate Model or Inaccurate Statistics of Dynamics? J. Phys. Chem. A 128, 6798–6805 (2024).
18. Chen, P.-Y.; Chen, Y.-C.; Chen, P.-P.; Lin, K.-T.; Sargsyan, K.; Hsu, C.-P.; Wang, W.-L.; Hsia, K.-C.; Ting, S.-Y. A Whole-Cell Platform for Discovering Synthetic Cell Adhesion Molecules in Bacteria. Nat Commun, 15, 6568 (2024).
19. Li, C.; Wei, T.-Y.; Cheung, M. S.; Tsai, M.-Y.* Deciphering the Cofilin Oligomers via Intermolecular Disulfide Bond Formation: A Coarse-Grained Molecular Dynamics Approach to Understanding Cofilin's Regulation on Actin Filaments. J. Phys. Chem. B, 128, 4590–4601 (2024).

Thematic Group 4.3 Complex Systems

Coordinator: Pik-Yin Lai (National Central University; Email: pylai@phy.ncu.edu.tw)

I. Brief Description

The Thematic Group TG4.3, focused on exploring the vast complexities of complex systems, is led by Dr. Pik-Yin Lai from National Central University (NCU). This group brings together experts from across Taiwan and beyond to unravel the intricate patterns and behaviors found in systems that span physics, biology, and complex systems. TG4.3's core team includes well-established scientists such as Hong-Yan Shih and Sheng-Hong Chen from Academia Sinica, Hsuan-Yi Chen from NCU, Cheng-Hung Chang from NYCU, Lee-Wei Yang and Guang-Ron Huang from NTHU. The group is supported by talented postdoc researchers, including Chia-Chou Wu and Koushik Goswami, who contribute fresh insights and energy to ongoing projects.

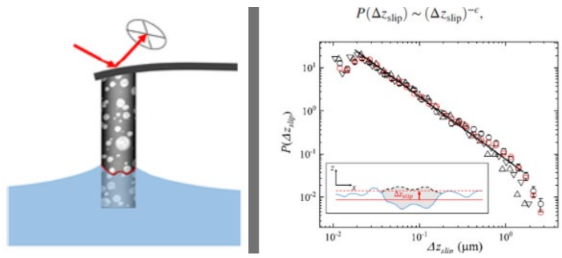
Through collaboration and cross-disciplinary projects, TG4.3 focuses on phenomena like non-equilibrium statistical mechanics, network dynamics, cell dynamics, non-linear systems, biophysics and bioinformatics that can reveal surprising insights into real-world applications. Their aim is not only to advance theoretical understanding but to open doors to practical solutions in fields ranging from biology, soft-materials, to artificial intelligence.

II. Activities

Over the past two years, TG4.3 has kept a lively schedule of activities that engages both group members and the broader scientific community:

TG4.3 hosted the annual Complex Systems Symposium and Frontiers of Complex Systems Winter School, focusing on specialized topics within non-equilibrium dynamics, biophysics and complex systems. These events provided an opportunity for scientists to dive deep into specific aspects of complex systems research, with a strong focus on real-world applications and emerging trends. In 2023, TG4.3 organized a satellite meeting as part of the 28th IUPAP International Conference on Statistical Physics, which brought together an enthusiastic community of over 125 participants from countries like Japan, Germany, the U.S., Italy, and the UK. The theme "Emergent Behavior in Biological Networks" attracted over 70 students eager to engage in dynamic discussions about how complex systems principles apply to biological systems. TG4.3 continues to promote collaboration through cross-TG workshops. A recent workshop held with TG4.2 delved into overlapping areas between physics, Chemistry and biological systems. These cross-group interactions are crucial for fostering new insights and breaking down traditional research boundaries, enabling participants to approach complex systems from fresh perspectives.

III. Visitors and International Collaborations



TG4.3 has actively fostered international collaborations and welcomed short-term visitors who bring diverse expertise to the group's research efforts. Recent collaborations include partnerships with leading institutions such as UC San Diego (UCSD), Niels Bohr Institute, and institutions in Japan and Denmark. Collaborations with UCSD and B. Hof's group on the role of stochasticity in turbulent transitions, which has already led to key publications in *Nature Physics*. Partnership with HKUST's Penger Tong, together with collaborations within

TG members (PY Lai and HY Chen) on projects exploring avalanche dynamics in liquid as well as solid interfaces, have led to publications in *Nature Communications* and *Physical Review Letter* (selected as Editor's Suggestions).

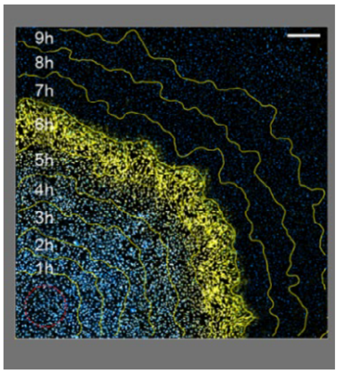
Dynamic International Exchanges: Over 17 international scientists have visited TG4.3 recently, contributing to ongoing research projects and participating in collaborative efforts across fields like statistical physics and complex biological networks. These visits have helped to solidify TG4.3's role as a nexus for high-impact research in Taiwan.

IV. Highlights of Research Results

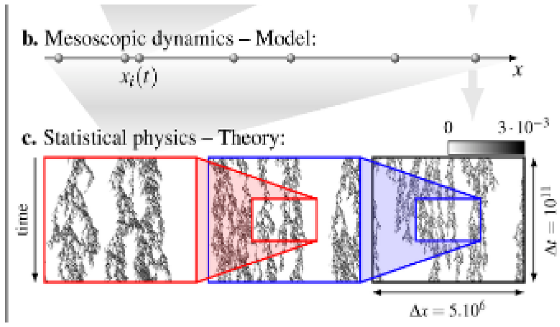
TG4.3 has seen significant advancements in several exciting research areas. Here are some of the key highlights:

● HY Chen (NCU) and PY Lai (NCU) collaborated with the experimental group in HKUST lead by Penger Tong on the non-equilibrium statistical mechanics of random pinning field under external drive. In particular, their join effort on the Statistical laws of stick-slip friction at mesoscale, led to a paper in *Nature Communications*. They further collaborated with and the experimental group in HKUST led by Penger Tong on Avalanches and extreme value statistics of a moving contact line led to a paper published in *Phys. Rev. Lett.* 2024. Their findings contained significant advances in the field and the paper was selected as the *Editor's Suggestions*.

● SH Chen and CC Wu (NCTS postdoc 2021~2023) worked on the dynamics of living cell, both experimentally and theoretically on the oscillatory response dynamics associated with p53, which leaded to a paper in *Cell* published in the end of 2022. They further worked on the emergence of large-scale cell death via trigger waves of ferroptosis, which led to a paper in *Nature* 2024.



● HY Shih (AS) collaborated with the experimental group of B. Hof, and theorist N. Goldenfeld (UCSD) on the role of stochasticity in the transition to turbulence in pipe flow and shear



flow, which led to a paper in *Nature Physics*.

● Statistical Mechanics of Colloidal Heat Engines: collaborations within TG members (CH Chang and HY Chen) led to development on colloidal heat engines driven by engineered active noise. Their research, published in Phys. Rev. Research, demonstrates how active noise can power microscopic engines, opening up new possibilities for energy harvesting on small scales.

● Applied Biophysics using Machine Learning: Lee-Wei Yang's team used advanced machine learning algorithms to analyze the intrinsic dynamics of proteins, shedding light on how these movements affect biological processes. Their work, which applies elastic network models to drug discovery, underscores the value of integrating physics-based theories with cutting-edge AI techniques led to a paper in *Current Opinion in Structural Biology*. Their work further showed that how deep learning methods for drug discovery benefit from protein dynamics data. In particular, they developed label-free triboelectric nanosensors for Anti-Tumor Drugs screening that led to a paper in *Nano Energy.*

- Stochastic Thermodynamics in Non-equilibrium Systems: PY Lai collaborated with local experimentalist Y. Jun, and yielded new insights into stochastic thermodynamics. Their study on a "gambling demon" strategy in non-equilibrium particle systems, featured in Phys. Rev. Research, illustrates how information on decision making can harness gain in free energy.
- Mechanosensitive Bonds and Cell Motility Patterns: Hsuan-Yi Chen's recent work explores how bonds within cells respond to mechanical forces, a discovery that could have significant implications for understanding cell migration and cancer metastasis. The findings, published in Phys. Rev. Research, are helping researchers' model how cells move in response to their environment.
- PY Lai collaborated with the theorist CH Cheng (NCUE) on constructing the theory of non-equilibrium asymptotic states, and also on the non-equilibrium thermodynamics of the Ehrenfest multi-urn model with interactions. Their joint effort has already leaded to several papers in past years (*Phys. Rev. E 2020, 2023, 2024; Phys. Rev. Res. 2021*) and their new theory on non-equilibrium asymptotic states has received very positive reviews.

TG4.3's activities over the past couple years have contributed substantial advancements to the field of complex systems, highlighting the power of collaboration and interdisciplinary research. With its dedicated team and growing international network, TG4.3 continues to push boundaries, making strides in both theoretical and experimental science. We look forward to the next phase of exploration and discovery!

V. (Selected) Publications (with NCTS as an affiliation only)

TG4.3's prolific research output over the past two years has included publications in high-impact journals. Below are a few selected papers that showcase the group's contributions:

- "Directed percolation and puff jamming near the transition to pipe turbulence",G. Lemoult, M. Vasudevan, H.-Y. Shih, G. Linga, J. Mathiesen, N. Goldenfeld and B. Hof, *Nat. Phys* 20, 1339 (2024)
- "Emergence of large-scale cell death via trigger waves of ferroptosis". Co H.K.C, Wu C.-C, Lee Y.-C, Chen S.-H. *Nature*. 2024 Jul;631(8021):654-662. PMID: 38987590 (Noted in: Waves of ferroptotic cell death sculpt embryonic tissue. Nature News and Views 2024 July 10)
- "Avalanches and extreme value statistics of a moving contact line", C. Yan, D. Guan, Y. Wang, H.Y. Chen*, Pik-Yin Lai*, P Tong*, *PR L* 132, 084003-1~6 (2024). (Editor's Suggestion)
- "Statistical laws of stick-slip friction at mesoscale", C. Yan, H.Y. Chen, Pik-Yin Lai, P. Tong, *Nature Communications* 14, 6221 (2023).
- "Colloidal Heat Engine Driven by Engineered Active Noise," Phys. Rev. Research (2023) by J.A.C. Albay, Z.Y. Zhou, C.H. Chang, H.Y. Chen, and Y. Jun.
- "Activity-Assisted Barrier-Crossing of Self-Propelled Colloids Over Parallel Microgrooves," Phys. Rev. E (Letter) (2023) by Y. Wen, Z. Li, H. Wang, J. Zheng, J. Tang, X.P. Xu, and P.Y. Lai.
- "Mechanosensitive Bonds Induced Complex Cell Motility Patterns," Phys. Rev. Research (2024) by J.-Y. Lo, Y.-H. Tseng, and H.Y. Chen.
- "Mutually beneficial confluence of structure-based modeling of protein dynamics and machine learning methods", Anupam Banerjee, Satyaki Saha, Nathan C. Tvedt, Lee-Wei Yang, Ivet Bahar, *Current Opinion in Structural Biology* 78, 102517 (2023).
- "Theory of Non-equilibrium Asymptotic State Thermodynamics: Interacting Ehrenfest Urn Ring as an Example," Phys. Rev. E (2024) by C.H. Cheng and P.Y. Lai.

III. Research Activities of Individuals

A. Articles from Center Scientists

Advances in Thermally-Assisted-Occupation DFT

Professor

Jeng-Da Chai

Deputy Director

National Taiwan University

Nanoscale Physics and Chemistry

Over the last 30 years, Kohn-Sham (KS) density functional theory (DFT) has been the most popular electronic structure method for predicting the electronic properties of large ground-state systems because of its decent balance between performance and cost. Nonetheless, since the existing exchange-correlation (xc) energy functionals are approximate, they can lead to qualitative failures in various situations. Consequently, developing a density functional method resolving these qualitative failures at an affordable computational cost is of tremendous importance.

Recently, we have proposed a DFT with fractional orbital occupations (governed by the Fermi-Dirac distribution with some fictitious temperature), i.e., thermally-assisted-occupation (TAO)-DFT [1] to explore the ground-state properties of large electronic systems with strong static correlation effects. Besides, we have also developed the semilocal [2] and global hybrid [3] functionals in TAO-DFT for an improved performance in a wide range of applications. In addition, we have developed a self-consistent scheme [4] to determine the fictitious temperature in TAO-DFT, which is generally superior in performance for a broad range of applications.

Very recently, we have proposed a simple model [5] to define the optimal system-independent fictitious temperature of a given energy functional in TAO-DFT. In addition, we have employed this model to determine the optimal system-independent fictitious temperature of a global hybrid functional in TAO-DFT as a function of the fraction of exact exchange. Furthermore, we have discussed the role of exact exchange and an optimal system-independent fictitious temperature in TAO-DFT.

To explore the equilibrium thermodynamic and dynamical properties of nanosystems with radical character at finite temperatures, we have recently combined TAO-DFT with *ab initio* molecular dynamics (AIMD), leading to TAO-DFT-based AIMD (TAO-AIMD) [6].

In our recent study [7], the orbital occupation numbers obtained from TAO-DFT have been shown to be qualitatively similar to the natural orbital occupation numbers obtained from an accurate multi-reference (MR) electronic structure method, leading to a similar trend for the radical character of various alternant polycyclic aromatic hydrocarbons.

To demonstrate the applicability of TAO-DFT, we have recently employed TAO-DFT to study the ground-state properties of various strongly correlated electron systems at the nanoscale (e.g., zigzag graphene nanoribbons [8] and many others), which have been regarded as challenging systems for conventional electronic structure methods (e.g., KS-DFT with conventional xc energy functionals).

Since 2023, we have made the following achievements related to TAO-DFT. First, to study solvation effects on the ground-state properties of nanomolecules with MR character at a minimal computational cost, we have recently combined TAO-DFT with the polarizable continuum model (PCM), leading to TAO-DFT-based PCM (TAO-PCM) [9]. In TAO-PCM, the solute is treated quantum-mechanically with TAO-DFT, and the solvation effect is modeled implicitly with the PCM. To show its usefulness, TAO-PCM has been adopted to study the electronic properties of linear acenes in three different solvents (toluene, chlorobenzene, and water).

Second, we have recently developed a real-time (RT) extension of TAO-DFT (RT-TAO-DFT) [10] based on an ensemble formalism. RT-TAO-DFT allows the study of time-dependent (TD) properties of both single-reference (SR) and MR systems. Since the assumption of a weak perturbation is not required in RT-TAO-DFT, spin-restricted and spin-unrestricted RT-TAO-DFT calculations have been performed to explore the TD properties (e.g., the number of bound electrons, induced dipole moment, and high-order harmonic generation (HHG) spectrum) of H2 at the equilibrium and stretched geometries, aligned along the polarization of an intense linearly polarized laser pulse. The TD properties obtained with RT-TAO-DFT have been compared with those obtained with conventional TD-DFT. Moreover, issues related to the possible spin-symmetry breaking effects in the TD properties are also discussed. Furthermore, for clarity, we have also discussed the difference among three generally different electronic structure methods: KS-DFT, TAO-DFT, and FT-DFT (finite-temperature density functional theory, also called the Mermin-Kohn-Sham (MKS) method) as well as TAO-DFT-related methods.

Third, we explored issues related to spin symmetry in TAO-DFT. For MR systems, KS-DFT with the traditional xc energy functionals can yield wrong spin densities and related properties. For instance, for the dissociation of H_2 and N_2, the spin-restricted and spin-unrestricted solutions obtained from the same xc energy functional in KS-DFT can be distinctly different, leading to the unphysical spin-symmetry breaking effects in the spin-unrestricted solutions. Very recently, we have developed a response theory [11] based on TAO-DFT to demonstrate that TAO-DFT with a sufficiently large fictitious temperature can always resolve the aforementioned spin-symmetry breaking problems (which are challenging problems for KS-DFT).

Fourth, we have used TAO-DFT to predict the electronic properties of graphene nano-parallelograms (GNPs) [12]. GNPs exhibit an oscillatory polyradical nature with increasing GNP length, and the polyradical nature is also highly dependent on the GNP width. The edge/corner localization of active orbitals has been observed for the wider and longer GNPs.

In addition, TAO-DFT has been recently used to study the electronic properties of acenes in oriented external electric fields (OEEFs), where the OEEFs of various electric field strengths are applied along the long axes of acenes [13]. The MR character of ground-state acenes in OEEFs increases with the increase in the acene length and/or the electric field strength.

References:

[1] J.-D. Chai, J. Chem. Phys. **136**, 154104 (2012).

[2] J.-D. Chai, J. Chem. Phys. **140**, 18A521 (2014).

[3] J.-D. Chai, J. Chem. Phys. **146**, 044102 (2017).

[4] C.-Y. Lin, K. Hui, J.-H. Chung, and J.-D. Chai, RSC Adv. **7**, 50496 (2017).

[5] B.-J. Chen and J.-D. Chai, RSC Adv. **12**, 12193 (2022).

[6] S. Li and J.-D. Chai, Front. Chem. **8**, 589432 (2020).

[7] C.-N. Yeh and J.-D. Chai, Sci. Rep. **6**, 30562 (2016).

[8] C.-S. Wu and J.-D. Chai, J. Chem. Theory Comput. **11**, 2003 (2015).

[9] S. Seenithurai and J.-D. Chai, Nanomaterials **13**, 1593 (2023).

[10] H.-Y. Tsai and J.-D. Chai, Molecules **28**, 7247 (2023).

[11] Y.-Y. Wang and J.-D. Chai, Phys. Rev. A **109**, 062808 (2024).

[12] S. Seenithurai and J.-D. Chai, Molecules **29**, 349 (2024).

[13] C.-Y. Chen and J.-D. Chai, Molecules **29**, 4245 (2024).

Charmed baryon decays, CP violation, Light scalar mesons, Lifetimes of heavy baryons

Adjunct Research Fellow

Hai-Yang Cheng

Honorary Center Scientist
Institute of Physics, Academia Sinica
Particle physics

1. There exist two distinct ways in realizing the approximate SU(3) flavor symmetry of QCD to describe the two-body nonleptonic decays of charmed baryons: the irreducible SU(3) approach (IRA) and the topological diagram approach (TDA). The TDA has the advantage that it is more intuitive, graphic and easier to implement model calculations. TDA was developed by Ling-Lie Chau, Ben Tseng and me in 1996 to describe hadronic charmed baryon decays. The data of 2-body charmed baryon decays have been accumulated to the extent that it is mature to perform a global fit. We have obtained the fitting branching fractions, decay parameters, magnitudes of S- and P-wave amplitudes and their phase shifts in both the TDA and IRA. These results can be tested in the near future (see 2414.01350, 2410.04675).

Our next goal is to explore direct CP violation (CPV) in the charmed baryon decays. According to the standard model, CPV is very small in the decays of charmed hadrons. This is because CPV in the charm sector is governed by the CKM matrix element $V_{ub}^*V_{cb}$ which is very tiny in magnitude. As Cheng Wei and I had pointed out in 2012 that final-state rescattering can generate a penguin topology whose long-distance effects can be inferred from the TDA. Indeed, we have predicted the CP asymmetry difference in $D^0 \to \pi^+\pi^-$ and $D^0 \to K^+K^-$ to be $\Delta A_{CP} = (-1.51 \pm 0.04)10^{-3}$. Amazingly, it is in good agreement with the LHCb's first observation of CPV in the charmed meson sector in 2019 with the result $\Delta A_{CP} = (-1.54 \pm 0.29)10^{-3}$. Therefore, a generalization of our idea to the charmed baryon decays will render it possible to enhance CPV from 10^{-4} to the per mille level. This work is now on going.

2. The underlying structure of the light scalar mesons $f_0(500), f_0(980), a_0(980), K_0^*(700)$, whether they are two-quark or tetraquark states, is not well established both experimentally and theoretically. Recently, Cheng-Wei Chiang, Fanrong Xu and I pointed out that the decays $D \to a_0(980)\pi$ serve a remarkable place for discriminating the internal structure of $a_0(980)$. If $a_0(980)$ is a $q\bar{q}$ state, the predicted branching ratios of $D \to a_0^+(980)\pi$ will be too small by one to two orders of magnitude compared to experiment, while the predicted rates for $D^+ \to a_0^0(980)\pi$ and $D^0 \to a_0(980)^-\pi$ are usually too large compared to the data. We have shown that these difficulties can be resolved in the tetraquark model of $a_0(980)$ as there exist additional T-like topological diagrams. Therefore, measurements of $D \to a_0(980)P$ decays lend strong support to the tetraquark nature of $a_0(980)$ (see 2408.13942).

3. In 2023 Chia-Wei Liu and I started to re-examine the lifetimes of heavy baryons. To appreciate the importance of this work, let me briefly introduce the background of this topic. The predicted lifetime hierarchy for charmed baryons in heavy quark expansion (HQE) is given by $\tau(\Xi_c^+) > \tau(\Lambda_c^+) > \tau(\Xi_c^0) > \tau(\Omega_c^0)$ which seemed to agree with the experimental observation for a long time. However, the situation was dramatically changed in 2018 when LHCb reported a new measurement of the charmed baryon Ω_c^0 lifetime using semileptonic b-hadron decays. LHCb found a new lifetime of Ω_c^0 which is nearly four times longer than the 2018 world-average value of $\tau(\Omega_c^0)$. As a result, a new lifetime pattern emerged $\tau(\Xi_c^+) > \tau(\Omega_c^0) > \tau(\Lambda_c^+) > \tau(\Xi_c^0)$. The LHCb observation of a huge jump of the Ω_c^0 baryon lifetime is very striking from both experimental and theoretical points of view. In 2017 and 2018 I have worked on the charmed baryon lifetimes to order $1/m_c^4$ in HQE and calculated the baryon matrix elements of dimension-6 and dimension-7 four-quark operators in the framework of non-relativistic quark model (NRQM). During the HIEPA Workshop held in Beijing in March 2018 before the LHCb experiment, I reported the preliminary result that Ω_c^0 could live longer than Λ_c^+ with a lifetime of order 230 fs due to the suppression from $1/m_c$ corrections arising from dimension-7 four-quark operators!

However, the NRQM has some difficulties, for example, the matrix element is proportional to the baryon wave function modulus squared at the origin $|\psi(0)|^2$. It is found this quantity for the charmed baryon is much less than that for the bottom baryon in the NRQM. This renders NRQM estimate questionable. To overcome this difficulty Chia-Wei and I employ an improved MIT bag model with the issue of CMM being removed to evaluate the matrix elements. The results are satisfactory and respect HQE. Consequently, we have an updated and accurate estimate of the charmed baryon lifetime, especially $\tau(\Omega_c^0)$ (see 2306.00665).

Chiral Symmetries in High Temperature QCD

Professor

Ting-Wai Chiu

Honorary Center Scientist
National Taiwan University
Lattice QCD, High Energy Phenomenology

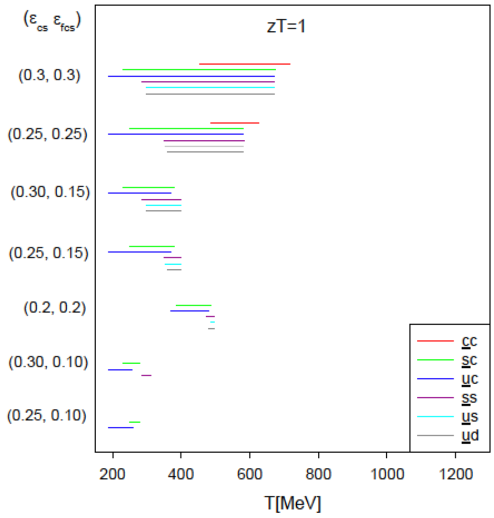
Understanding the nature of strongly interacting matter at high temperatures is crucial for uncovering the mechanisms governing matter creation in the early universe and elucidating the outcomes of relativistic heavy ion collision experiments such as those at LHC and RHIC, as well as those of electron ion collision experiments at the planned electron-ion colliders. A first step in this pursuit is to find out the symmetries in quantum chromodynamics (QCD) at high temperatures, which are essential in determining the properties and dynamics of matter under extreme conditions.

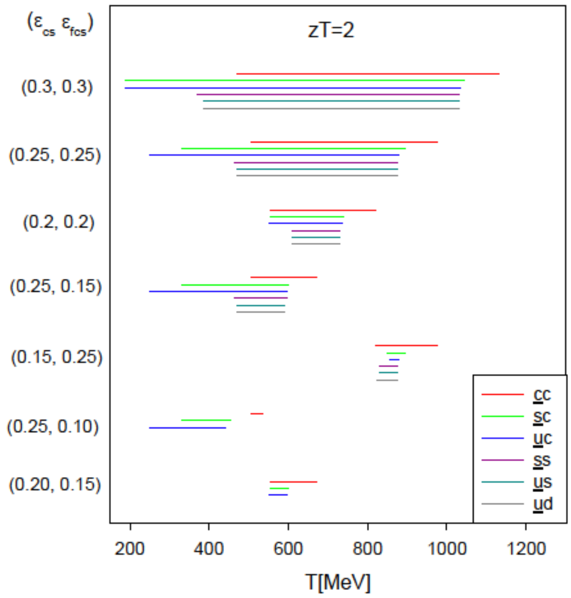
In the last two years, I have been studying the chiral symmetries of high temperature QCD by simulations of lattice QCD with $(\mathrm{u}, \mathrm{d}, \mathrm{s}, \mathrm{c})$ quarks at the physical point [1,2]. One of the interesting results of my study is the hierarchical restoration of chiral symmetries as the temperature is increased successively from low to high temperatures, from $SU(2)_L \times SU(2)_R \times U(1)_A$ of (u, d) quarks to $SU(3)_L \times SU(3)_R \times U(1)_A$ of $(\mathrm{u}, \mathrm{d}, \mathrm{s})$ quarks, then to $SU(4)_L \times SU(4)_R \times U(1)_A$ of $(\mathrm{u}, \mathrm{d}, \mathrm{s}, \mathrm{c})$ quarks. This is the first result of lattice QCD. One of the phenomenological implications of the hierarchical restoration of chiral symmetries is the pattern of hadron dissolution at high temperatures, which leads to the hierarchical dissolution of hadrons, and the hierarchical suppression of hadrons in the quark-gluon plasma. In other words, the hierarchy of dissolution of mesons of different flavors is exactly the same as that of the restoration of chiral symmetries, i.e.,

$$T^{\bar{u}d} < T^{\bar{u}s} < T^{\bar{u}c} < T^{\bar{s}s} < T^{\bar{s}c} < T^{\bar{c}c}$$

This leads to the hierarchical suppression of mesons in quark-gluon plasma, which could be observed in the relativistic heavy ion collision experiments such as those at LHC and RHIC.

Besides the hierarchical restoration of chiral symmetries, I also studied whether there are any (approximate) emergent symmetries which are not the symmetries of the entire QCD action but only a part of it, e.g., the $SU(2)_{CS}$ chiral spin symmetry (with $U(1)_A$ as a subgroup) which is only a symmetry of chromoelectric part of the quark-gluon interaction, and also the color charge. Since the free fermions as well as the chromomagnetic part of the quark-gluon interaction do not possess the $SU(2)_{CS}$ symmetry, its emergence in high temperature QCD suggests the possible existence of hadronlike objects which are predominantly bound by chromoelectric interactions. In [2], I first observed that the temperature windows for the emergence of $SU(2)_{CS}$ symmetry are dominated by the channels of heavy vector mesons with flavor contents $(\bar{u}\mathrm{c}, \bar{s}\mathrm{c}, \bar{c}\mathrm{c})$, as shown in Fig. 1.





Here $(\epsilon_{cs}, \epsilon_{fcs})$ are $SU(2)_{CS}$ symmetry breaking and fading parameters, with the smaller value having the higher precision of the $SU(2)_{CS}$ symmetry. These are the first results of lattice QCD. The emergence of approximate $SU(2)_{CS}$ symmetry suggests that these hadronlike objects, in particular, in the channels of vector mesons with the charm quark, at the temperatures inside their T windows, are likely to be predominantly bound by the chromoelectric interactions into color singlets. Moreover, this provides hints to look for the approximate emergent $SU(2)_{CS}$ symmetry in the relativistic heavy ion collision experiments such as those at LHC and RHIC, e.g., to focus on the channels of vector mesons with the charm quark.

[1] T.W. Chiu, Symmetries of meson correlators in high-temperature QCD with physical (u/d, s, c) domain-wall quarks, Phys. Rev. D 107, 114501 (2023).

[2] T.W. Chiu, Symmetries of spatial correlators of light and heavy mesons in high temperature lattice QCD, Phys. Rev. D 110, 014502 (2024).

Quantum Computing and its Interdisciplinary Applications

Professor

Hsi-Sheng Goan

Center Scientist

National Taiwan University

Quantum Computing and Quantum Information

Quantum computing represents a paradigm shift in the way we process and analyze information, offering tremendous potential for interdisciplinary applications across various fields. We describe some of the results we have obtained regarding quantum computing and its potential applications, including quantum error correction [1,2], quantum computational chemistry [3], quantum machine learning [4], and quantum gate operation and analysis [5].

Quantum Error Correction:

- **Counting stabilizer codes for arbitrary dimension**

This work was done in collaboration with Dr. Tanmay Singal at the Nicolaus Copernicus University in Poland, who was a former postdoctoral fellow of TG1.1. In this work, we compute the number of $[[n, k]]_d$ stabilizer codes made up of d-dimensional qudits for arbitrary positive integers d. Our work makes available this quantifier for the generic case, and thus is an important step needed to place results for quantum computing with non-prime dimensional quantum systems on the same pedestal as prime-dimensional systems [1].

- **Existence of Pauli-like stabilizers for every quantum error-correcting code**

This work was done with my postdoc, Dr. Jhih-Yuan Kao. The Pauli stabilizer formalism is perhaps the most thoroughly studied means of procuring quantum error-correcting codes, whereby the code is obtained through commutative Pauli operators and "stabilized" by them. In this work we will show that every quantum error-correcting code, including Pauli stabilizer codes and subsystem codes, has a similar structure, in that the code can be stabilized by commutative "Paulian" operators which share many features with Pauli operators and which form a *Paulian stabilizer group*. By facilitating a controlled gate, we can measure these Paulian operators to acquire the error syndrome. Examples concerning codeword stabilized codes and bosonic codes will be presented; specifically, one of the examples has been demonstrated experimentally and the observable for detecting the error turns out to be Paulian, thereby showing the potential utility of this approach. This work provides a possible approach to implement error-correcting codes and to find new codes [2].

Quantum Computational Chemistry: Accurate Harmonic Vibrational Frequencies for Diatomic Molecules via Quantum Computing

This is an on-going work in collaboration between the TG 1.1 core members, Jyh-Pin Chou, Yuan-Chung Cheng, and Hsi-Sheng Goan as well as Alice Hu at City University of Hong Kong. During the noisy intermediate-scale quantum (NISQ) era, quantum computational approaches refined to overcome the challenge of limited quantum resources are highly valuable. A comprehensive benchmark for a quantum computational approach in this spirit could provide insights toward further improvements. On the other hand, the accuracy of the molecular properties predicted by most of the quantum computations nowadays is still far off (not within chemical accuracy) compared to their corresponding experimental data. In this work, we propose a promising qubit-efficient quantum computational approach and present a comprehensive investigation by benchmarking quantum computation of the harmonic vibrational frequencies of a large set of neutral closed-shell diatomic molecules with results in great agreement with their experimental data. To this end, we construct the accurate Hamiltonian using molecular orbitals, derived from density functional theory to account for the electron correlation and expanded in the Daubechies wavelet basis set to allow an accurate representation in real space grid points, where an optimized compact active space is further selected so that only a reduced small number of qubits is enough to yield an accurate result [3].

Typically, calculations achieved with 2 to 12 qubits using our approach would need 20 to 60 qubits using traditional cc-pVDZ basis set with frozen core approximation to achieve similar accuracy. To justify the approach, we benchmark the performance of the Hamiltonians spanned by the selected molecular orbitals by first transforming the molecular Hamiltonians into qubit Hamiltonians and then using the exact diagonalization method to calculate the results, regarded as the best results achievable by quantum computation to compare to the experimental data. Furthermore, using the variational quantum eigensolver algorithm with the constructed qubit Hamiltonians, we show that the variational quantum circuit with the chemistry-inspired UCCSD ansatz can achieve the same accuracy as the exact diagonalization method except for systems whose Mayer bond order indices are larger than 2. For those systems, we then demonstrate that the heuristic hardware-efficient RealAmplitudes ansatz, even with a substantially shorter circuit depth, can provide significant improvement over the UCCSD ansatz, verifying that the harmonic vibrational frequencies could be calculated accurately by quantum computation in the NISQ era [3].

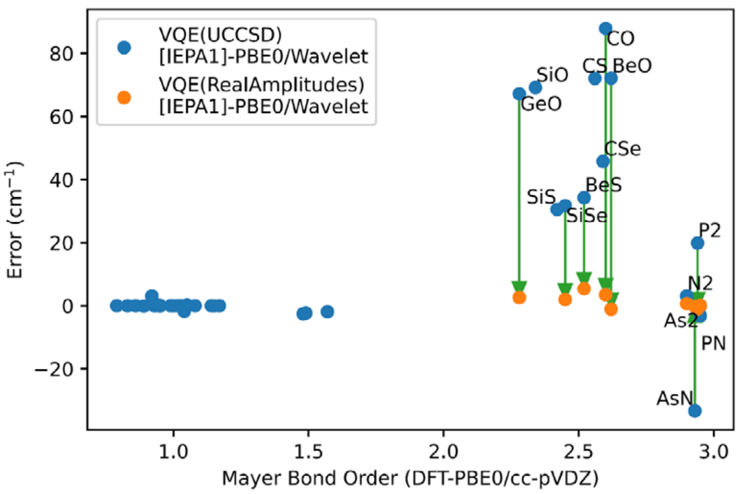


Fig. 1. Mayer bond order indices versus the error (difference) in the harmonic vibrational frequencies (in cm^{-1}). The orange dots denote the vibrational frequency results for the specified molecules calculated by RealAmplitudes ansatz while the blue dots by UCCSD ansatz. The green arrows point toward the directions of improvement from the UCCSD ansatz to the RealAmplitudes ansatz.

Quantum Machine Learning (QML):

- **Quantum Train: A novel hybrid quantum-classical machine learning approach**

We introduce the quantum-train (QT) framework, a novel approach that integrates quantum computing with classical machine learning algorithms to address significant challenges in data encoding, model compression, and inference hardware requirements. Even with a slight decrease in accuracy, QT achieves remarkable results by employing a quantum neural network alongside a classical mapping model, which significantly reduces the parameter count from M to O(polylog(M)) during training. Our experiments demonstrate QT's effectiveness in classification tasks, offering insights into its potential to revolutionize machine learning by leveraging quantum computational advantages. This approach not only improves model efficiency but also reduces generalization errors, showcasing QT's potential across various machine learning applications [4].

Quantum Gate Operation and Analysis:

- **Hamiltonian Phase Error in Resonantly Driven CNOT Gate Above the Fault-Tolerant Threshold**

This work is done with my Ph.D. student, Yi-Hsien Wu who is currently conducting experimental work in silicon-based quantum-dot spin qubits in Prof. S. Taruch's group in RIKEN and we provide theory support for this experimental work. Electron spin qubits are a promising platform for scalable quantum processors because of their long coherence time and compatibility with industrial foundry processes, A full-fledged quantum computer will need quantum error correction, which requires high-fidelity quantum gates. Analyzing and mitigating the gate errors are useful to improve the gate fidelity. Here, we demonstrate a simple yet reliable calibration procedure for a high-fidelity controlled-rotation gate in an exchange-always-on Silicon quantum processor allowing operation above the fault-tolerance threshold of quantum error correction. We find that the fidelity of our uncalibrated controlled-rotation gate is limited by coherent errors in the form of controlled-phases and present a method to measure and correct these phase errors. We then verify the improvement in our gate fidelities by randomized benchmark and gate-set tomography protocols. Finally, we use our phase correction protocol to implement a virtual, high-fidelity controlled-phase gate [5].

References:

1. Tanmay Singal, Che Chiang, Eugene Hsu, Eunsang Ki, **Hsi-Sheng Goan**, and Min-Hsiu Hsieh, "Counting stabilizer codes for arbitrary dimension", Quantum **7**, 1048 (2023).
2. Jhih-Yuan Kao and **Hsi-Sheng Goan**, "Existence of Pauli-like stabilizers for every quantum error-correcting code", Physical review A **108**, 032414 (2023).
3. S.-K. Chou, J.-P. Chou, A. Hu, Y.-C. Cheng*, and **Hsi-Sheng Goan** *, "Accurate Harmonic Vibrational Frequencies for Diatomic Molecules via Quantum Computing", Physical Review Research **5**, 043216 (2023)
4. C.-Y. Liu*, E.-J. Kuo*, C.-H. A. Lin, J. G. Young, Y.-J. Chang, M.-H. Hsieh*, **Hsi-Sheng Goan***, Quantum-Train: Rethinking Hybrid Quantum-Classical Machine Learning in the Model Compression Perspective, arXiv:2405.11304.
5. Y.-H. Wu*, L. C. Camenzind, A. Noiri, K. Takeda, T. Nakajima, T. Kobayashi, C.-Y. Chang, A. Sammak, G. Scappucci, **Hsi-Sheng Goan**, and S. Tarucha*, "Hamiltonian Phase Error in Resonantly Driven CNOT Gate Above the Fault-Tolerant Threshold", npj Quantum Information **10**, 8 (2024).

Harnessing Light-Matter Interactions for Quantum Reservoir Engineering

Assistant Professor

Chiao-Hsuan Wang

Center Scientist

National Taiwan University

Quantum Computation, Information, and Optics Theory

Quantum Reservoir Engineering

Quantum systems are inherently vulnerable to environmental influences. Quantum reservoir engineering aims to transform traditionally detrimental interactions between quantum systems and their environment into useful resources [1], with broad applications in quantum computation, state preparation, entanglement generation, metrology, simulation, and error correction. By carefully controlling the coupling between the system and its reservoir, additional effects such as non-Markovian behavior and unique thermodynamic properties in heat engines can also be achieved.

Squeezed Thermal Reservoir

One intriguing type of reservoir is the squeezed thermal reservoir [2]. Squeezing, a quantum phenomenon that reduces fluctuations in one phase-space quadrature while increasing them in the conjugate quadrature, is a powerful resource in quantum information science with broad implications across various fields of physics. Quantum systems coupled to squeezed reservoirs can exhibit compelling behaviors, such as extended atomic lifetimes and anomalous resonance fluorescence. Squeezed reservoirs also provide unique opportunities for generating dissipative squeezing and stabilizing entanglement.

We present a novel method for engineering squeezed thermal reservoirs using only linear, time-independent interactions [3]. Unlike previous approaches relying on nonlinear interactions, squeezed light injections, or time-dependent modulations, our method eliminates these complexities, offering a practical framework for experimental implementation across diverse quantum systems. The effectiveness of our reservoir engineering scheme is demonstrated through two key examples: extending qubit lifetimes and achieving dissipative cavity squeezing.

Extending Qubit Lifetime

By coupling a qubit (such as an atom or superconducting qubit) to a lossy cavity, we demonstrate the ability to emulate the dynamics of a qubit decaying into a squeezed thermal reservoir. This engineered environment enables direct control over the squeezing strength and angle through adjustments to the system's physical parameters. Simulations reveal a pronounced difference in qubit lifetimes along two transverse directions on the Bloch sphere: the decay rate is exponentially suppressed along the x-direction due to reduced environmental fluctuations, thereby extending the qubit's lifetime, at the expense of exponentially enhanced decay along the y-direction, as illustrated in Fig. 1. This phenomenon highlights the effectiveness of our squeezed thermal reservoir engineering method and its potential to extend qubit lifetimes.

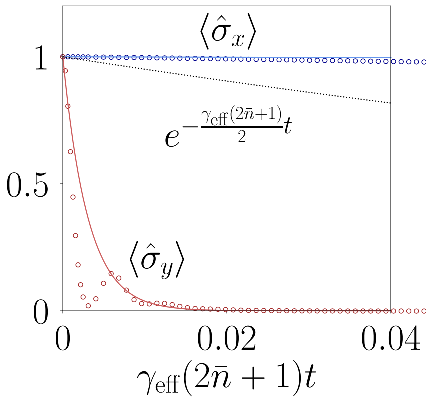


Figure 1: Simulated qubit dynamics inside the squeezed thermal reservoir, showing decay rate suppression along the x-direction and enhancement along the y-direction [3].

Dissipative Cavity Squeezing

We can engineer a squeezed thermal reservoir for bosonic systems, such as photons or phonons, to achieve dissipative squeezing in the steady state. By coupling a photonic cavity to a lossy cavity, the system experiences both a squeezing Hamiltonian and squeezed dissipation. With suitable parameters, it reaches a steady state with significant squeezing. In Figure 2, the Wigner function of the steady state displays a distinct elliptical distribution in phase space, highlighting the strong squeezing effect and validating our reservoir engineering scheme.

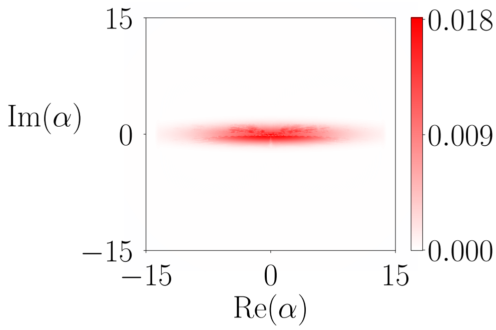


Figure 2: Wigner function of the system cavity's steady state, illustrating strong squeezing with an elliptical phase-space distribution [3].

Our work demonstrates an experimentally feasible approach to engineering squeezed thermal reservoirs, requiring no nonlinear squeezed light inputs or time-dependent modulations, and paves the way for advanced quantum technologies with broad implications across diverse fields of physics.

[1] J. F. Poyatos, J. I. Cirac, and P. Zoller, Phys. Rev. Lett. 77, 4728 (1996).
[2] C. W. Gardiner and M. J. Collett, Phys. Rev. A 31, 3761 (1985).
[3] C.-L. Lee and C.-H. Wang, arXiv:2408.16052 (2024), under review.

Error Analysis in Quantum Communication Networks

Associate Professor

Hao-Chung Cheng

Center Scientist

National Taiwan University

Quantum Information Theory

In quantum information science, transmitting classical information over a noisy quantum channel is a foundational task. To protect the transmitted messages against potential quantum noise, I have developed a simple, effective, and physically-implementable coding strategy based on the so-called pretty-good measurement. The approach sharpens and streamlines the previously known achievable error bounds. Moreover, the proposed technique does not rely on certain structural hypotheses of the underlying quantum channel, such as independent and identical noises, and hence it applies to general non-correlated or non-stationary quantum channels. The derived one-shot capacities for unassisted and entanglement-assisted classical communication over quantum channels are both the tightest heretofore. One-shot error bounds for various quantum network information-processing protocols are also covered in a unified manner. The established error bounds are tighter than previously known, and the derivation is *simpler*, *technically innovative*, and more *conceptually intuitive*. The strength, simplicity, and variability of the derived error characterizations make the proposed coding and analysis likely a textbook approach when studying classical communication in one-shot and asymptotical quantum information theory. The established decoding technique to is expected to yield further applications in other fields of quantum information and technology. The single-authored paper [1] was accepted and presented at the most *premier* quantum information science conference – *26th Conference on Quantum Information Processing* (QIP, February 4-10, 2023, Ghent, Belgium) – as the ***short plenary talk***. Later, [1] is published in *PRX Quantum*.

Discriminating and testing entangled quantum states under quantum operations with locality constraints is one of the most technical challenging problems in quantum information science and quantum networking. In the paper [2] published in *Communication in Mathematical Physics*, we first proposed a mathematical framework to address this question and establish tight exponential error bounds for testing arbitrary *multipartite entangled pure quantum state* against its orthogonal complement.

We investigated the asymptotic inclusion relations between three important quantum operation classes – Local Communication with Classical Communication (LOCC), Separable (SEP) operations, and Positive Partially-Transposed (PPT) operations. We established a sufficient and necessary condition of when the three classes collapse. We showed that testing maximally entangled and extremal Werner states fulfill the above condition, and hence have derived their *exact characterization* of the optimal error probability in hypothesis testing. Our findings are surprising because the LOCC protocols could achieve similar performance as the PPT operations even when testing *highly entangled states*.

Lastly, we proposed a novel measure to quantify the *unextendibility* of a product basis and we established its *multiplicativity* property. This mathematical technique yields a quantitative proof for a remarkable result: Tensor product of unextendible product bases (UPB) is still an UPB. Based on this, we demonstrated an *infinite separation* between the SEP and PPT operations by an example constructed from UPBs. This finding demonstrates an even more striking and counter-intuitive phenomenon because there is no entanglement involved in the UPB example, yet SEP could be substantially restricted compared to the PPT class.

In summary, the work [2] provides two new techniques and concepts to lower bound the error probability in asymptotical quantum state discrimination: (a) a succinct dual formula for the PPT-distinguishability norm; and (b) an unextendibility measure, which are of significance in distributed quantum state discrimination.

Privacy amplification against quantum adversaries is a crucial primitive in quantum cryptography (such as Quantum Key Distribution) and quantum information-theoretic security. A central question is: What is the maximal extractable randomness for an ε -extractor? When using the so-called purified distance as a security criterion, an almost optimal one-shot characterization has been established by Tomamichel and Hayashi [*IEEE Trans. Info. Theory 59 (11), 2013*]. Nevertheless, the *trace distance* is the most relevant security criterion in cryptography due to the physical indistinguishability and composability. Hence, an almost optimal one-shot extractable randomness under trace distance was remained open prior to our work. In the paper [3], we have solved this 10-year open problem by characterizing the one-shot maximal extractable randomness in terms of the so-called (1-ε) conditional hypothesis-testing entropy (which is computable via a semi-definite program). Our achievability error analysis *quadratically improves* upon the existing results. Moreover, the established result is tight in the sense that it yields the optimal second-order rates in the scenario of independently and identically prepared sources.

This work was first accepted and presented at *26th Conference on Quantum Information Processing* (QIP, February 4-10, 2023, Ghent, Belgium) as a contributed talk, and later published in *IEEE Transactions on Information Theory*.

In the paper [4] published in *IEEE Transactions on Information Theory*, we studied the quantum soft covering problem – how many quantum states are sufficient to approximate a given target state? This task is fundamental to distributed source simulation, wiretap channel coding, identification, and lossy data compression. We have established a one-shot achievable error exponent and proved a one-shot strong converse bound. The achievability bound strictly improves upon all the previously known results and hence could immediately sharpen the above-mentioned quantum information-processing tasks.

Interestingly, our result yields a novel concentration inequality for random operators under trace norm, which can be viewed as a quantum generalization of the well-known Markov inequality in classical probability theory. The established fundamental technique could be of independent interest in Mathematical Physics.

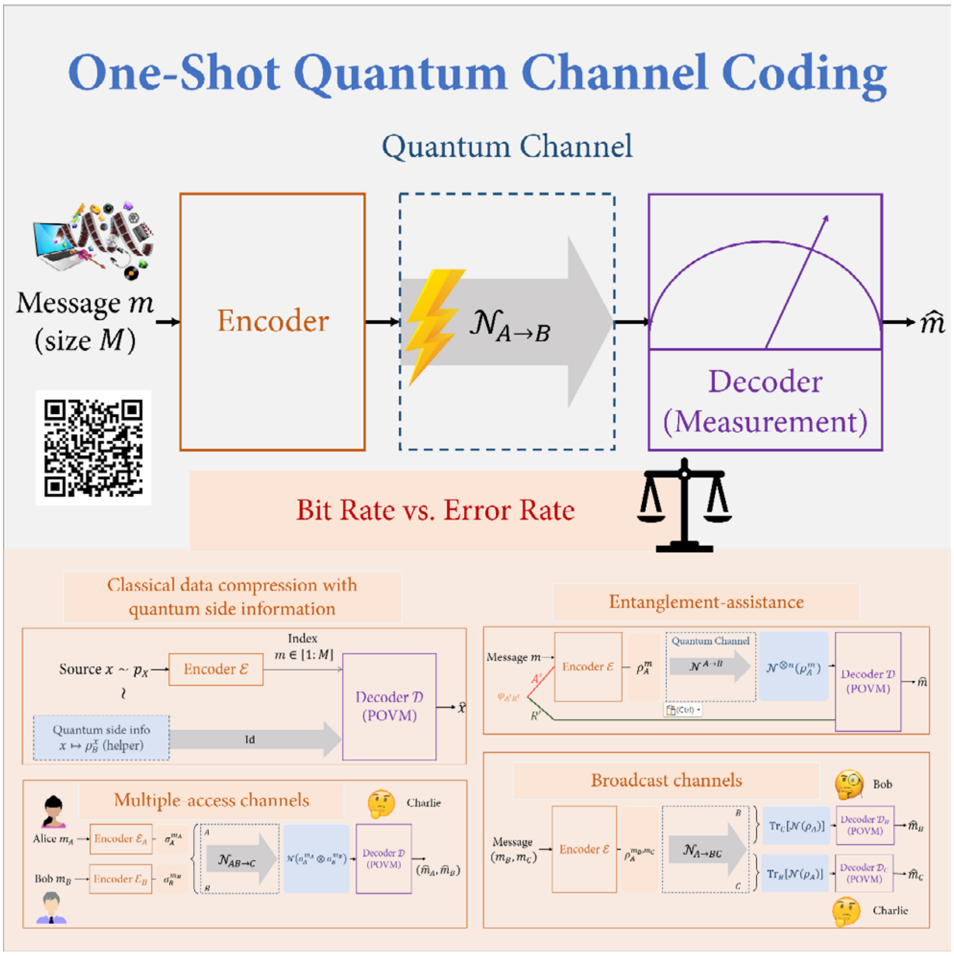


Fig. 1: An illustration of one-shot channel coding over quantum noisy channels. The aim is to design a proper encoding and decoding strategy for various types of quantum communication channels for possibly multiple senders and receivers.

Aside from quantum information theory, we also made significant to an important topic of quantum compilation in quantum computing. In the paper [5] published in *ACM Transactions on Quantum Computing*, we studied the so-called Qubit Mapping problem, a critical aspect of implementing quantum circuits on real hardware devices. Currently, the existing algorithms for qubit mapping encounter difficulties when dealing with larger circuit sizes involving hundreds of qubits. In this article, we introduce an innovative qubit mapping algorithm, Duostra, tailored to address the challenge of implementing large-scale quantum circuits on real hardware devices with limited connectivity. Duostra operates by efficiently determining optimal paths for double-qubit gates and inserting SWAP gates accordingly to implement the double-qubit operations on real devices. Together with two heuristic scheduling algorithms, Limitedly Exhaustive Search and Shortest-Path Estimation, it yields results of good quality within a reasonable runtime, thereby striving toward achieving quantum advantage. Experimental results showcase our algorithm's superiority, especially for large circuits beyond the NISQ era. For example, on large circuits with more than 50 qubits, we can reduce the mapping cost by an average 21.75% over the previously known best results. Furthermore, our method can handle problem sizes up to 11,969-qubit QFT within 3 hours (with time complexity $O(n^{2.8})$, where n denotes the numbers of qubits). In summary, our proposed qubit mapping framework offers a solution for large-scale quantum circuits by efficiently implementing local-optimal quantum algorithms on a non-fully connected quantum device.

[1] **Hao-Chung Cheng***, "Simple and Tighter Derivation of Achievability for Classical Communication Over Quantum Channels," *PRX Quantum*, 4, 040330, 22 November, 2023.

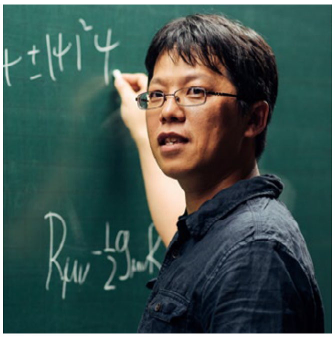
[2] **Hao-Chung Cheng***, Andreas Winter, and Nengkun Yu, "Discrimination of Quantum States Under Locality Constraints in the Many-Copy Setting," *Communications in Mathematical Physics*, 404:151-183, 14 September 2023.

[3] Yu-Chen Shen, Li Gao, **Hao-Chung Cheng***, "Optimal Second-Order Rates for Quantum Soft Covering and Privacy Amplification," *IEEE Transactions on Information Theory*, Volume: 70, Issue: 7, July 2024.

[4] **Hao-Chung Cheng*** and Li Gao, "Error Exponent and Strong Converse for Quantum Soft Covering," *IEEE Transactions on Information Theory*, Volume: 70, Issue: 5, May 2024.

[5] Chin-Yi Cheng, Chien-Yi Yang, Yi-Hsiang Kuo, Ren-Chu Wang, **Hao-Chung Cheng***, Chung-Yang (Ric) Huang, "Robust Qubit Mapping Algorithm via Double-Source Optimal Routing on Large Quantum Circuits," *ACM Transactions on Quantum Computing*, Volume 5, Issue 3, Pages 1–26, 2024.

Quantum Machine Learning: Applications to Metrology and Gravitational Wave Detectors



Professor

Ray-Kuang Lee

Center Scientist

National Tsing Hua University

Quantum Optics, Gravitational Wave Detectors

We implement machine-learning (ML) enhanced quantum state tomography (QST) for continuous variables, through the experimentally measured data generated from squeezed vacuum states, as an example of quantum machine learning. Our recent progress is applying such a ML-QST as a crucial diagnostic toolbox for applications including Wigner currents, optical cat state generation, and Bayesian estimation for the advanced gravitational wave detectors.

Machine-Learning Enhanced Quantum State Tomography for the Gravitational Wave Detectors

AI-generated image of a quantum robotic Schrödinger's cat that reads a quantum machine learning review paper.

Fig. 1: Review on Machine learning with a quantum robotic cat reading our review paper [1].

Quantum machine learning is a rapidly growing field at the intersection of quantum technology and artificial intelligence. In 2023, we were invited for a Review article on Quantum Machine Learning [1], emphasizing on a two-fold overview of several key approaches that can offer advancements in both the development of quantum technologies and the power of artificial intelligence.

The implementation of our machine-learning (ML) enhanced quantum state tomography (QST) for continuous variables, through the experimentally measured data generated from squeezed vacuum states, are demonstrated as an example of quantum machine learning [2]. In addition to quantum sensors [3], such a ML-QST is proposed as a crucial diagnostic toolbox for applications with squeezed states for the advanced gravitational wave detectors [4,5], through the collaborations with LIGO-Virgo- KAGRA (LVK) gravitational wave network and Einstein Telescope.

As one application, we also experimentally reconstruct Wigner's current of quantum phase-space dynamics [6]. We reveal the "push-and- pull" associated with damping and diffusion due to the coupling of a squeezed vacuum state to its environment. In contrast to classical dynamics, where (at zero temperature) dissipation only "pulls" the system toward the origin of phase space, we also observe an outward "push" because our system must obey Heisenberg's uncertainty relations.

Experimental Realization of Optical Cat States with Photon-Added Squeezed States:

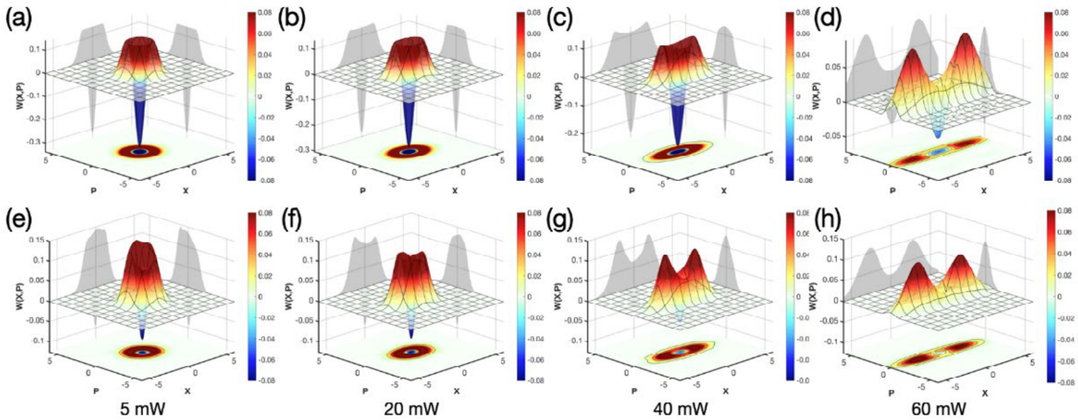


Fig. 2: Wigner distributions of our optical cat states: (a–d) for the theoretical photon-added squeezed states, and (e–h) for experimental data with 92% detection efficiency correction.

As one application, we also experimentally reconstruct Wigner's current of quantum phase-space dynamics [6]. We reveal the "push-and- pull" associated with damping and diffusion due to the coupling of a squeezed vacuum state to its environment. In contrast to classical dynamics, where (at zero temperature) dissipation only "pulls" the system toward the origin of phase space, we also observe an outward "push" because our system must obey Heisenberg's uncertainty relations.

Regarding optical cat states, the non-classical superposition of two quasi-classical coherent states, we report the first experimental realization of optical 'cat states' by adding a photon to a squeezed vacuum state, so far only photon-subtraction protocols have been realized [7]. Photon-addition gives us the advantage of using heralded signal photons as experimental triggers, and we can generate 'cat states' at rates exceeding 2.3×10^5 counts per second. Our most highly squeezed vacuum input state shows -8.9 dB squeezing, but such squeezing entails some degradation, in this case, 15.1 dB anti-squeezing. Even so, our approach enables us to synthesize a state with a maximum 'cat amplitude' of $|\alpha| \approx 1.77$ whose Wigner distribution still shows pronounced negative parts. Our experimental implementation with controlled photon-addition demonstrates a new powerful building block for advanced quantum state synthesis.

References:

[1]. Alexey Melnikov, Mohammad Kordzanganeh, Alexander Alodjants, and RKL," Quantum Machine Learning: from physics to software engineering," **Advances in Phys. X** (Review Article) 8, 2165452 (2023) [51 pages].

[2]. Hsien-Yi Hsieh, Yi-Ru Chen, Hsun-Chung Wu, Hua Li Chen, Jingyu Ning, Yao-Chin Huang, Chien-Ming Wu, and RKL, "Extract the Degradation Information in Squeezed States with Machine Learning," **Phys. Rev. Lett.** 128, 073604 (2022).

[3]. Dmitriy Tsarev, Stepan Osipov, RKL,

Sergey Kulik, and Alexander Alodjants, "Quantum sensor network metrology with bright solitons," **Phys. Rev. A** 108, 062612 (2023).

[4]. RKL, "Machine-learning enhanced quantum state tomography and quantum noise reduction to the advanced gravitational wave detectors, " **Proc. of SPIE** 12912, 1291213 (2024); Quantum Sensing, Imaging, and Precision Metrology II, SPIE Quantum West, San Francisco, California, United States, Jan. 27- Feb. 1, 2024 (Invited talk).

[5]. RKL, "KAGRA upgrade plans," LIGO-Virgo-KAGRA Collaboration Meeting, Barcelona, September 22nd – 27th, 2024 (Plenary talk).

[6]. Yi-Ru Chen, Hsien-Yi Hsieh, Jingyu Ning, Hsun-Chung Wu, Hua Li Chen, You-Lin Chuang, Popo Yang, Ole Steuernagel, Chien-Ming Wu, and RKL, "Experimental reconstruction of Wigner phase-space current," **Phys. Rev. A** 108, 023729 (2023).

[7]. Yi-Ru Chen, Hsien-Yi Hsieh, Jingyu Ning, Hsun-Chung Wu, Hua Li Chen, Zi-Hao Shi, Popo Yang, Ole Steuernagel, Chien-Ming Wu, and RKL, "Generation of heralded optical `Schrödinger cat' states by photon-addition," **Phys. Rev. A** 110, 023703 (2024).

Two-Dimensional Schrödinger Simulator using Electromagnetically induced Transparence

Professor

Wen-Te Liao

Center Scientist

National Central University

Quantum Optics

In our publication [1], we investigate a two-dimensional electromagnetically induced transparence (EIT) system [1] as presented in Fig. 1. The system is based on a two-dimensional setup of three-level Λ-type atoms (Fig.1a), which exhibits three distinct quantum states: $|1\rangle$, $|2\rangle$, and $|3\rangle$. Fig.1b shows that the transitions between these atomic states, specifically $|1\rangle \rightarrow |3\rangle$ and $|2\rangle \rightarrow |3\rangle$, are driven by external control lasers Ω_c^i and probe lasers Ω_p^i, where $i = F, B, R,$ and L indicating forward, backward, rightward, and leftward, respectively. Δ_c and Δ_p are the detuning of control and probe fields, respectively. We found it can be effectively described by the following Schrödinger-like equation

$$i\hbar\frac{\partial\rho_{21}}{\partial t} = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_T + \vec{A}\right)^2\rho_{21} + U\rho_{21} + i\left(\frac{\Gamma}{2\Delta_\mathrm{p}}\right)\frac{\hbar^2}{2m}\nabla_T^2\rho_{21}.$$

Here ρ_{21} is the quantum coherence between two states $|1\rangle$ and $|2\rangle$ and plays the key role in the neutral quasi particle called dark state polariton (DSP) in EIT physics. $\vec{A}$ and U are effective vector and scalar potentials. Inspired by the above Schrödinger-like equation, we design a method to generates synthetic gauge potentials for dark-state polaritons (DSPs) using the Landau gauge in a controlled laboratory environment. This is a crucial element in creating controllable quantum phenomena such as Landau levels and edge states for DSPs. One of the most striking observations in our system is the presence of Landau levels in DSPs. Landau levels, typically observed in charged particles under a magnetic field, manifest here due to the synthetic gauge potential, confirming the system's ability to mimic magnetic effects in a neutral atomic setup. Additionally, as depicted by Fig.1(c), we observed robust edge states further solidifying the potential of this system to emulate complex quantum phenomena in a fully controlled manner. The key advantage of our system is its all-field nature, meaning it relies entirely on the interaction between light and atoms to achieve the synthetic gauge potential. This all-optical approach opens the door to manipulating DSPs in ways that would be impossible using mechanical or magnetic techniques. The versatility of light fields allows for dynamic control, enabling the realization of quantum simulations and devices with a higher degree of precision and flexibility. For example, by tuning the properties of the control and probe lasers, it is possible to adjust the synthetic gauge potential and alter the energy landscape of the DSPs.

Looking ahead, our research aims to build on these promising results in several key areas. One of our immediate goals is to explore non-Hermitian systems within this framework. Non-Hermitian systems, which include dissipative processes or interactions with the environment, have been shown to exhibit unique quantum effects that differ from traditional Hermitian systems. By introducing controlled loss mechanisms or incoherent processes, we hope to uncover novel phenomena in DSPs that are inaccessible in standard Hermitian models.

[1] Y.-H. Kuan et al., Phys. Rev. Research 5, L042029 (2023).

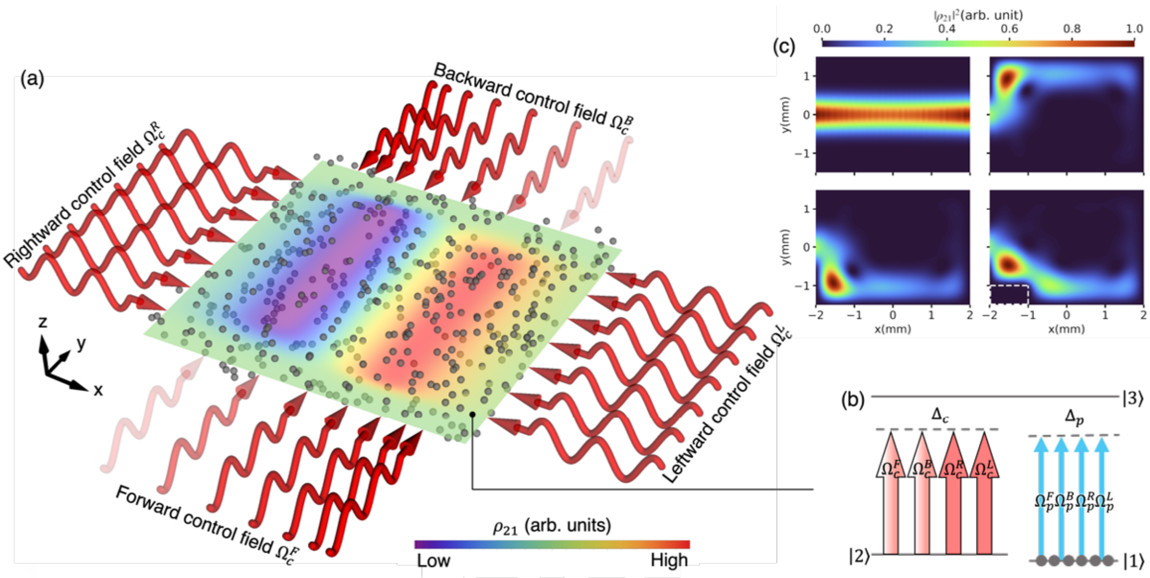


FIG. 1: (a) Two-dimensional Schrödinger simulator using EIT. Gray dots represent atoms, and the red-sinusoidal arrows illustrate control fields. The density and the opacity of arrows reflect the control field strength. The coloured density plot depicts the spatial distribution of the dark-state coherence ρ_{21}. (b) three-level system (three atomic states $|1\rangle$, $|2\rangle$, and $|3\rangle$) coupled to four pairs of strong control (weak probe) fields Ω_c^i (Ω_p^i), where $i = F, B, R,$ and L indicating forward, backward, rightward, and leftward, respectively. Δ_c and Δ_p are the detuning of control and probe fields, respectively. (c) Robust DSP edge state under different effective magnetic fields. The dashed square shows the region of vacuum as an obstacle for the EIT slow light.

Quantum correlations on the nonsignaling boundary: characterization and applications

Professor

Yeong-Cherng Liang

Center Scientist

National Cheng Kung University

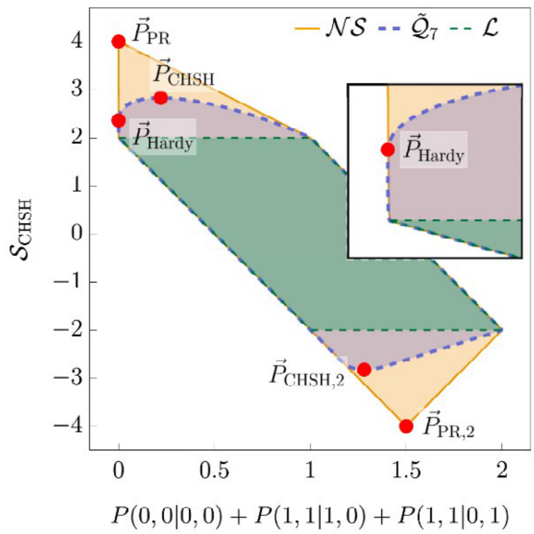
Quantum Information and Communication

One of the most striking features of quantum theory is that it allows for correlations between local measurement outcomes that defy Reichenbach's principle of (classical) common cause. Such correlations manifested in a Bell test are indispensable in device-independent (DI) quantum information, where one makes *no* assumption about the internal workings of the devices involved but deduces their nature directly from the observed measurement statistics.

Even though it is long-known that in a Bell test, the set of correlations allowed in quantum theory Q lies *strictly* between the Bell-local set L (constrained by the principle of local causality) and the no-signaling set NS (constrained by relativistic causality), many questions concerning the geometry of the quantum set remain unanswered. For example, when do the boundaries of Q and NS coincide? And when they coincide, do correlations lying on the common boundary allow for the possibility of self-testing, i.e., for one to conclude unambiguously that the underlying state and measurements leading to these correlations are essentially unique?

In [1], we resolve entirely this characterization problem in the simplest Bell scenario, where two parties can each perform two dichotomic measurements. Our findings show that modulo the freedom of relabeling, nonclassical, common boundaries of Q and NS fall within six different Classes, as specified by the number of zero entries in the correlation table and their relative positions. We further prove that self-testing is possible in all nontrivial Classes beyond the known examples of Hardy-type correlations. We also provide numerical evidence supporting the robustness of these self-testing results.

In addition, our findings suggest that all these self-testing quantum correlations found on the NS boundary are non-exposed. An example of that is given by $\vec{P}_{\text{Hardy}}$ shown below.



Notice that a non-exposed correlation in Q can never serve as the unique maximizer of a Bell inequality. This fact complicates the potential application of these extremal, Bell-nonlocal correlations in DI cryptographic tasks such as randomness generation, as we subsequently show in [3]. However, our complete characterization has also led to the discovery of a potential simplification over existing DI quantum key distribution protocols, which we are currently investigating in collaboration with leading experimental teams abroad.

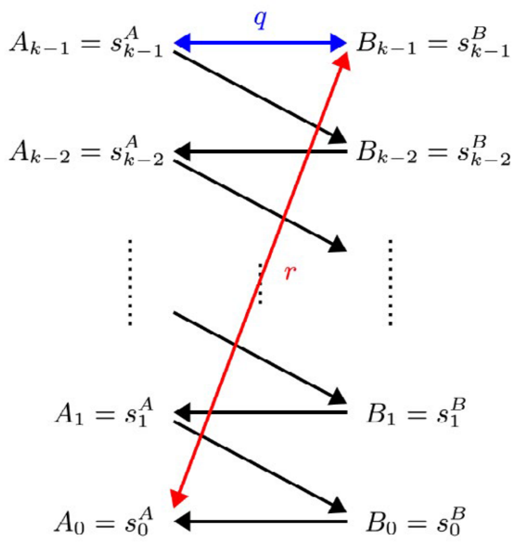
Finally, note that our findings in [1] have also led to our discovery [4] of generalizations of the so-called Hardy-type paradoxes for an arbitrary symmetric bipartite Bell scenario. The figure below schematically illustrates the logical structure underlying one such generalization via the failure of the transitivity of implications.

[1] K.-S. Chen, G. N. M. Tabia, C. Jebarathinam, S. Mal, J.-Y. Wu, and Y.-C. Liang, Quantum correlations on the no-signaling boundary: self-testing and more, *Quantum* **7**, 1054 (2023).

[2] K. T. Goh, J. Kaniewski, E. Wolfe, T. Vértesi, X. Wu, Y. Cai, Y.-C. Liang, and V. Scarani, Geometry of the set of quantum correlations, *Phys. Rev. A* **97**, 022108 (2018).

[3] C.-Y. Chen, K.-S. Chen, K.-M. Chung, M.-H. Hsieh, Y.-C. Liang, and G. N. M. Tabia, Incorporating Zero-Probability Constraints to Device-Independent Randomness Expansion, *arXiv:2401. 08452* (2024).

[4] K.-S. Chen, S. Mal, G. N. M. Tabia, and Y.-C. Liang, Hardy-type paradoxes for an arbitrary symmetric bipartite Bell scenario, *Phys. Rev. A* **109**, 042206 (2024).



Deep learning the hierarchy of steering measurement settings of qubit-pair states

Associate Professor

Hong-Bin Chen

Center Scientist

National Cheng Kung University

Quantum information and quantum computation

The quantum correlations between spatially separated parties are widely acknowledged as a nontrivial resource showing advantages over the classical counterparts for quantum foundations and quantum information. Among the family of quantum correlations, Bell nonlocality [1] is arguably the most famous one due to the historical debate of Einstein-Podolsky-Rosen paradox [2]. A nonlocal state can be certified by the violation of Bell's inequality [3], and can be explicitly applied to the fully device-independent quantum information tasks.

Apart from the fully device-independent scenario, the constraints can be relaxed to the one-side device-independent quantum information tasks, in which one of the two-party system (say Bob) is steered by the other party's (say Alice) untrusted measurements. In this Alice-to-Bob steering scenario, one relies on a steerable correlation, also referred to steerable assemblage, as a resource to achieve quantum advantages over an unsteerable assemblage admitting the local-hidden-state (LHS) models [4-6]. Such a quantum resource requires a steerable state with an incompatible measurement such that the generated assemblage is incompatible with the LHS models.

There have been many approaches to test the incompatibility of a given assemblage with respect to the LHS models; in contrast, to verify the steerability of a quantum state remains a cumbersome task. To that aim, one has to optimize over all possible incompatible measurements, e.g., (1) the number n of observables and (2) which observables to be measured on a given state. With this construction, the classification of quantum states according to the minimal number n of required observables to exhibit the steerability forms a hierarchy, which we refer to as the hierarchy of steering measurement settings.

There are some attempts to tackle this difficulty by deriving feasible criteria. For example, the criterion, derived by Bowles, Hirsch, Quintino, and Brunner (BHQB) [7], is a sufficient condition for verifying the qubit-pair unsteerability. Furthermore, the maximal violation of the steering inequality, derived by Cavalcanti, Jones, Wiseman, and Reid (CJWR) [8], by a qubit-pair state under 2 and 3 observables has been utilized as a quantifier of qubit-pair steerablity [9]. However, both conditions are not strong enough in fully discriminating the (un)steerability of qubit-pair states. The explicitly experimental examination of the insufficiency has been reported recently [10].

Here we leverage the power of the supervised deep learning algorithm to infer the fine-grained hierarchy of steering measurement settings. Due to the aforementioned insufficiency of the theoretical criteria, to exactly verify this hierarchy for quantum states is difficult, rendering the actual boundaries of the hierarchy undetermined. Such a problem without ground truth (GT), or hard to find out the ground truth, is called to be GT-deficient. This hinders the generation of reliable training data, as well as the training of a supervised deep learning algorithm.

To overcome this insufficiency, we construct a computational protocol by iteratively testing the steerability of a given qubit-pair state with the semidefinite program (SDP) under n random observables, designating the state to be n-measurement steerable (n-MS). This constitutes the necessary data set for training a deep learning algorithm.

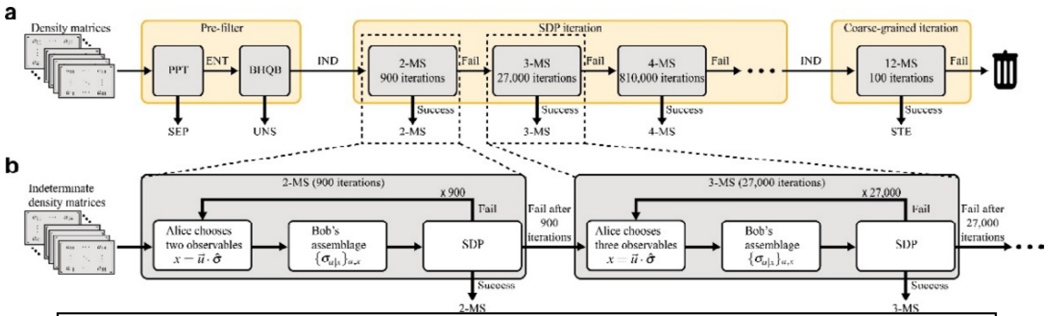


FIG. 1. Computational protocol generating the labeled training data.

Physical intuition on the steerability allows us to reduce the parameters encoding a qubit-pair state in the data set. From the counterintuitive responses of the well-trained deep learning models to the physics-driven parameters, we can acquire a compact, and precise, way for the characterization of steerability. Our results suggest that, in contrast to the entanglement, the characterization of the steerability from Alice to Bob is dominantly determined by Alice's regularly aligned ellipsoid; whereas Bob's ellipsoid is irrelevant. Recall that Alice's steering ellipsoid is defined to be the set of all states that can be steered to from Bob, and vice versa. Comparing these operational definitions of quantum steering and the steering ellipsoid, our results are seemingly counterintuitive. Therefore, we have also provided an explanation with the one-way stochastic local operations and classical communication (1W-SLOCC).

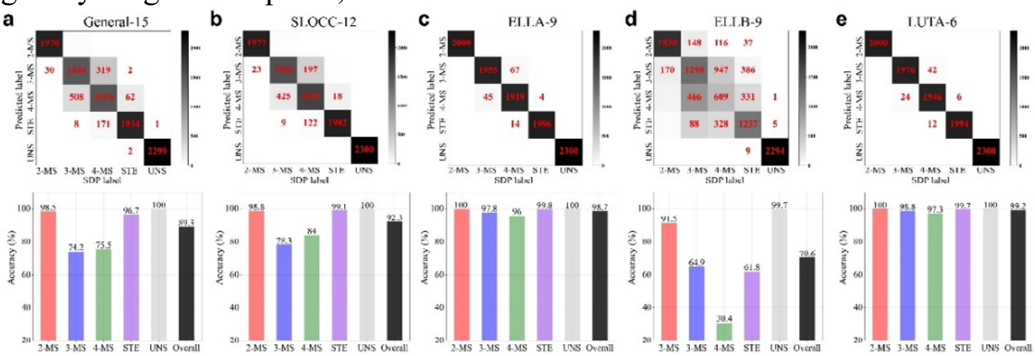


FIG. 2. Verification of the well-trained models on the testing data set.

For a comprehensive visualization, we have also applied the well-trained deep learning models to depict the hierarchy of two types of states generalized from the Werner state. Our models are capable of identifying the 4-MS states, i.e., the states requiring at least four observables to exhibit steerability on Bob, with high precision. Currently, no theoretical criteria in the literature are capable of efficiently determining the 4-MS states. Furthermore, with a different way of parameterizing the qubit-pair states, our models can also be applied to characterize hidden quantum steerability of generalized Werner states, whereby an unsteerable state becomes steerable after an 1W-SLOCC operation. Our results, on the one hand, unravel a new direction in the characterization of steerability; on the other hand, these also underpin the capability of the deep learning approaches to shed light on a new route toward the physics remaining obscure, rather than merely being a substitution of cumbersome computational tasks. Our results have been published in Ref. [11].

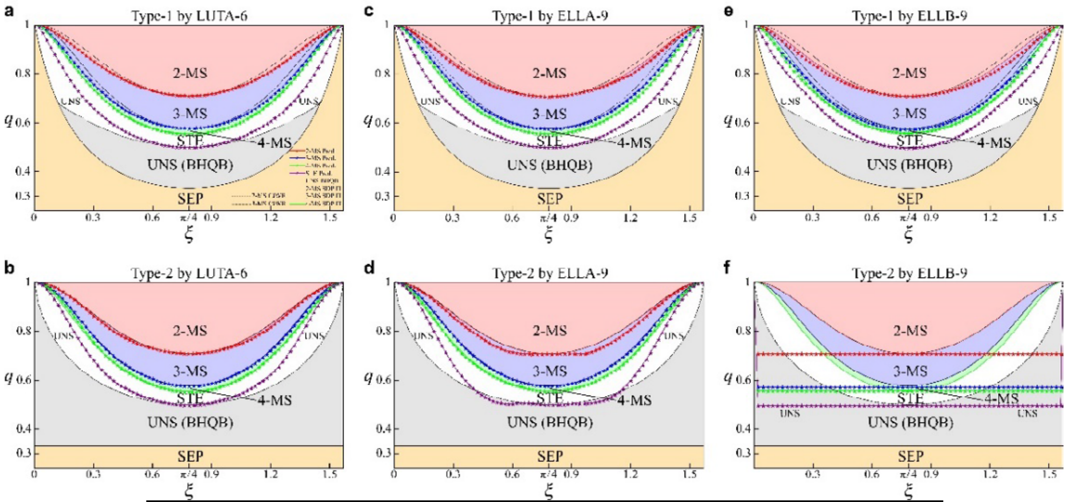


FIG. 3. Prediction of the hierarchy of both types of states.

[1] N. Brunner, D. Cavalcanti, S. Pironio, V. Scarani, and S. Wehner, Bell nonlocality, Rev. Mod. Phys. 86, 419 (2014).

[2] A. Einstein, B. Podolsky, and N. Rosen, Can quantum-mechanical description of physical reality be considered complete? Phys. Rev. 47, 777 (1935).

[3] J. S. Bell, On the Einstein Podolsky Rosen paradox, Physics 1, 195 (1964).

[4] H. M. Wiseman, S. J. Jones, and A. C. Doherty, Steering, Entanglement, Nonlocality, and the Einstein-Podolsky-Rosen Paradox, Phys. Rev. Lett. 98, 140402 (2007).

[5] D. Cavalcanti and P. Skrzypczyk, Quantum steering: a review with focus on semidefinite programming, Rep. Prog. Phys. 80, 024001 (2017).

[6] R. Uola, A. C. S. Costa, H. C. Nguyen, and O. Gühne, Quantum steering, Rev. Mod. Phys. 92, 015001 (2020).

[7] J. Bowles, F. Hirsch, M. T. Quintino, and N. Brunner, Sufficient criterion for guaranteeing that a two-qubit state is unsteerable, Phys. Rev. A 93, 022121 (2016).

[8] E. G. Cavalcanti, S. J. Jones, H. M. Wiseman, and M. D. Reid, Experimental criteria for steering and the Einstein-Podolsky-Rosen paradox, Phys. Rev. A 80, 032112 (2009).

[9] A. C. S. Costa and R. M. Angelo, Quantification of Einstein-Podolsky-Rosen steering for two-qubit states, Phys. Rev. A 93, 020103 (2016).

[10] K. Jiráková, A. Černoch, K. Lemr, K. Bartkiewicz, and A. Miranowicz, Experimental hierarchy and optimal robustness of quantum correlations of two-qubit states with controllable white noise, Phys. Rev. A 104, 062436 (2021).

[11] H.-M. Wang, H.-Y. Ku, J.-Y. Lin, and H.-B. Chen, Deep learning the hierarchy of steering measurement settings of qubit-pair states, Commun. Phys. **7**, 72 (2024)

Semi-Device-Independently Characterizing Quantum Temporal Correlations

Assistant Professor

Shin-Liang Chen

Center Scientist

National Chung Hsing University

Quantum Information Theory

Key Background

Classically, Bell's theorem outlines restrictions on the correlations predicted by local hidden-variable models, where correlations reflect quantum features unique to quantum mechanics. This concept, termed quantum non-locality, distinguishes quantum systems from classical ones and has practical implications for quantum certification methods, where non-locality can verify quantum properties without in-depth device details. This device-independence (DI) is especially valuable in real-world applications where the devices are often uncharacterized.

In addition to spatial non-locality (as discussed in Bell's theorem), researchers have explored temporal correlations, where non-macrorealistic behaviors emerge over time instead of across space. For instance, the Leggett-Garg scenario investigates non-classical temporal correlations, where a quantum state evolves through a series of measurements in time. Expanding this idea, the temporal Bell scenario considers various measurement choices at each time point, resembling spatial Bell tests in a temporal context. The focus here is to verify if observed statistics can be reproduced by quantum states and measurements in a temporal setup. However, characterizing these correlations in a DI or semi DI manner has been challenging.

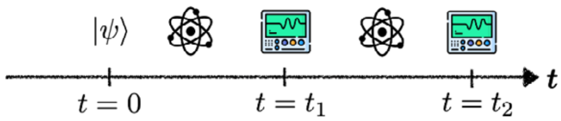


Fig. 1 The temporal scenario considered in this work.

The Instrument Moment Matrix (IMM) Framework

We introduce IMMs [1] to systematically capture quantum temporal correlations in temporal Bell scenarios. An IMM consists of a matrix formed from the post-measurement states' expectation values. If these states and their measurements align with quantum mechanics principles, the IMMs exhibit positive semi-definiteness. This matrix-based structure allows temporal quantum correlations to be processed using semi-definite programming, which has proven effective in similar hierarchical structures within quantum mechanics.

IMMs function effectively in both fully DI and semi-DI contexts. For the latter, IMMs permit incorporating partial device knowledge to create a more nuanced understanding of quantum states. This flexibility enables the framework to accommodate varied physical constraints, such as: 1) **No-Signaling-in-Time (NSIT)**, 2) **Dimensional Constraints**, and 3) **Rank Constraints**.

Applications and Implications

IMMs open several avenues for evaluating quantum resources and tasks under different constraints:

1. **Temporal Bell Inequalities**: We can use IMMs to compute the maximal quantum violation of a temporal Bell inequality.
2. **Temporal Steerability**: We can use the IMMs to evaluate the degree of temporal steerability in a DI way. Together with a recent work exploring the link between temporal steering and thermolization [2], we are also able to estimate the thermolization time of a system.
3. **Quantum Randomness Access Codes (QRACs)**: We can use the IMMs to compute the maximal successful probability of a scenario of quantum randomness access code.
4. **Self-Testing in Prepare-and-Measure**: We can use the IMMs to certify, in a DI way, a set of quantum states in a prepare-and-measure scenario.

Summary

This work advances quantum temporal correlation studies by establishing the IMM framework for characterizing correlations in a temporal Bell setup. The IMM approach's device-independent structure supports various constraints, making it suitable for tasks like measuring temporal steerability, testing temporal Bell inequalities, and performing quantum self-testing. IMMs provide practical methods for quantum information applications, including randomness access codes and thermalization measurements, underscoring their potential for advancing quantum certification and security technologies.

The IMM framework's versatility bridges a vital gap between fully device-independent and semi-device-independent settings, addressing real-world challenges in quantum experiments and quantum information security.

[1] Semi-Device-Independently Characterizing Quantum Temporal Correlations
Shin-Liang Chen and Jens Eisert
Phys. Rev. Lett. 132, 220201 (2024).

[2] Thermodynamic Approach to Quantifying Incompatible Instruments
Chung-Yun Hsieh and **Shin-Liang Chen***
Phys. Rev. Lett. 133, 170401 (2024).

Professor

Cheng-Wei Chiang

Center Scientist

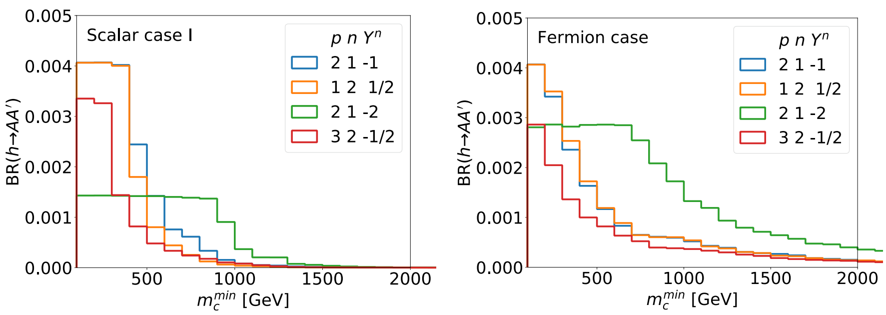
National Taiwan University

Particle Phenomenology

Within the two years (2023-2024) of being a Center Scientist, I have worked on projects in a few different directions: dark photon physics, deep machine learning techniques, phenomenology of exotic Higgs bosons, and flavor physics, among others. In the following, I select four papers to highlight our findings.

In **Phys. Rev. Lett. 130 (2023) 14, 141801**, we examined constraints on models allowing the Higgs boson to decay into **a photon and a massless dark photon** (h → A A'). Our analysis incorporates theoretical bounds such as unitarity and perturbativity, alongside experimental constraints from the oblique parameters, the Higgs signal strengths, and the electron electric dipole moment. These additional constraints and updated data make our results more robust, precise and stringent than previous phenomenological studies. The branching ratio BR(h → A A') was found to be limited to **0.4%**, as shown in Fig. 1, under constraints from Higgs signal strengths, electron electric dipole moments, oblique parameters, and unitarity. We also found an approximate relation between the above branching ratio and those of the measured diphoton and invisible decay modes of the Higgs boson, again confirming our strong upper bound. This limit was well below the bound found by other phenomenological studies by more than a factor of 10 and also better than the collider bound of **1.8%** (which was very recently improved to 1.3% in August 2024). The bound would be even stronger if the exotic **light charged particles** that mediate the process become heavier. Additionally, achieving a sizable branching ratio demands **large couplings** and introduces **Landau poles** at low energies, indicating that the models lack aesthetic simplicity and robustness.

Figure 1 Upper bound on the branching ratio as a function of the exotic charged particle mass, for a scalar case (left) and a fermion case (right)



Given the fact that the LHC and even the HL-LHC environment cannot achieve the required precision for this particular decay mode to test our upper bound, our work urges the experimental group to re-evaluate their search strategy or to improve the analysis techniques. Because of this paper, I was awarded the **2024 Sun Yat Sen Academic Writings Award** for

Natural Sciences.

In **Phys. Rev. D 107 (2023) 1, 016014**, we explored advanced machine learning techniques for distinguishing **vector boson fusion (VBF)** from **gluon-gluon fusion (GGF)** Higgs boson production. Building on previous studies, we compared **event-level deep learning classifiers** using low-level inputs, such as full-event images and particle 4-vectors, with models based on high-level physics features like jet kinematics and shapes. Our results demonstrated that CNN-based classifiers outperform shallow networks, achieving **significantly higher background rejection**, especially when additional jets and unclustered hadronic activity are incorporated, as shown in Fig. 2.

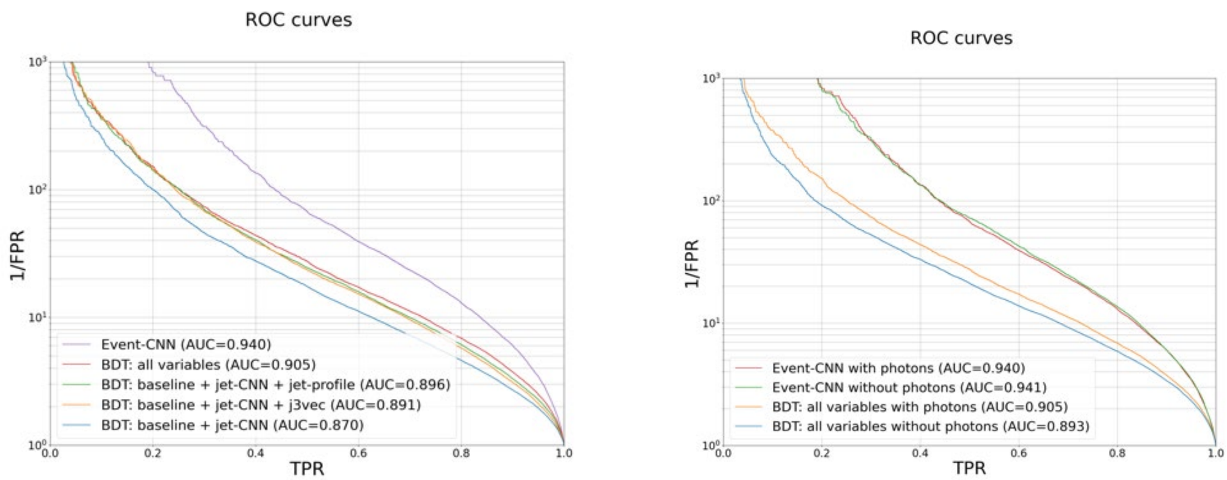


Figure 2 Performance comparison among different models (left) and performance with or without the diphoton information (right).

In the study, we also investigated why CNNs perform better by analyzing **saliency maps**, which revealed that event-level CNNs captured features beyond just the two leading jets, including subtle hadronic activity. We also experimented with adding these high-level jet features to the shallow networks, observing some performance improvements but confirming that **CNNs remained superior**. The study takes a step further by proposing a **decay-agnostic classifier**—a model that maintains performance even without using specific Higgs decay products, such as diphotons, as shown in the plot on the right.

Finally, we outlined several future directions, including developing **multiclass classifiers** for other Higgs production modes (e.g., ZH, WH, and ttH), studying newer architectures like **graph networks**, and incorporating **Lorentz-invariant symmetries** into network designs. This work provides an essential foundation for **decay-independent event-level classification** to streamline Higgs analysis across multiple decay modes.

In **JHEP 06 (2023) 069**, we explored an **extension of the Georgi-Machacek (GM) model** that introduces a **CP-violating (CPV) phase** into the Higgs potential. The study derives theoretical constraints, including vacuum stability, perturbative unitarity, and contributions to electric and neutron electric dipole moments (eEDM, nEDM). A key finding was that gauge-loop and charged-

Higgs-loop diagrams contributed significantly to the eEDM, though cancellations ensure compatibility with experimental bounds.

Moreover, we analyzed how CP-mixing between neutral scalars (H_1, H_2) influenced decay patterns into hZ and ZZ. When the CPV phase in the model increases, CP mixing enhances the branching ratios for these decays. Simulations indicate that the H_1 and H_2 mediated processes could potentially be detected at the HL-LHC. However, processes involving the heavier scalar H_3 were predicted to remain beyond current experimental sensitivity.

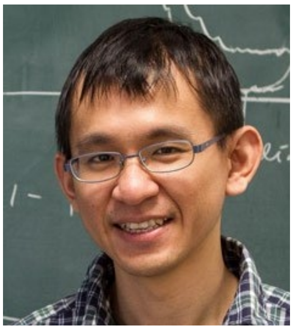
We presented **benchmarks for collider studies** that vary the CPV phase and analyze their impact on cross-sections for $gg \rightarrow H_{1,2} \rightarrow hZ \rightarrow bbZ$. The **future LHC runs at 14 TeV** could provide direct evidence of CP violation in the model. Additionally, deviations in Higgs decay patterns, particularly in the diphoton channel, could further distinguish this model from the **Standard Model (SM)** and **two-Higgs-doublet models (2HDMs)**.

More recently in **Phys. Rev. D 109 (2024) 7, 073008**, we provided an updated analysis of two-body decays, including $D \rightarrow$ PP, VP, and VV, using the **topological diagram approach** that make use of the flavor symmetry among the three light quarks. We discussed how interference between Cabibbo-favored (CF) and doubly Cabibbo-suppressed (DCS) decays affects asymmetries, such as those in K_S^0-K_L^0 mixing.

In the VP sector, we predicted deviations in strong phases and highlighted new puzzles from recent BESIII data, including unexpected dominance of higher partial waves. Currently, it is somewhat challenging to extract reliable helicity and partial-wave amplitudes due to limited data.

Another goal was to estimate the D^0-$\bar{D}^0$ mixing parameter y using the information of two-body decay branching ratios. We found that CF, DCS, and singly Cabibbo-suppressed (SCS) terms contribute to cancellations, leading to a small value for y. We estimated that at least half of the mixing parameter y can be accounted for by the PP and VP decay modes, though uncertainties remain due to incomplete measurements of DCS channels and unknown phase factors.

Supernova neutrinos, quantum kinetics, and dark matter



Associate Research Fellow

Meng-Ru Wu

Center Scientist

Institute of Physics, Academia Sinica

Astroparticle physics

Neutrinos, despite their weakly interacting nature, play a pivotal role in Nature's most catastrophic explosions that signify the death of massive stars – the core-collapse supernova explosions, and greatly influence the synthesis of elements therein [1]. The state-of-the-art theoretical modeling of supernova explosions taking into account all four fundamental forces, including general relativity, nuclear equation of state, neutrino interactions, as well as magnetic fields are being modeled through sophisticated numerical simulations that require millions of CPU hours are being developed. These models aim not only to explain various direct and indirect observations, but also to provide multimessenger prediction for the next galactic supernova event, which serves as a once-in-a-lifetime chance for greatly advancing our understanding across a wide range of important questions in astrophysics, nuclear physics, and particle physics.

However, it has recently been realized that a key physics ingredient, the flavor oscillations of neutrinos, which is not included in current supernova modeling, can largely affect our theoretical understanding of supernova explosions. For modeling this missing piece of physics, it requires solving the neutrino quantum kinetic equation, which is essentially a generalized Boltzmann transport equation including the quantum nature of neutrinos in the flavor space. This introduces a new physics scale of sub-centimeter in space (sub-nanosecond in time), originated from the forward scattering potential of neutrinos. As this intrinsic scale is several orders of magnitude smaller than those associated with other classical processes such as advection and collisions, the involved scale separation represents a significant challenge to the modeling of supernovae, which requires novel methods to overcome.

During the past few years, we have tried to develop advanced understanding of this problem and formulated a new framework that can help solve this problem [2-6]. By leveraging the scale separation nature of the problem, we first studied the behavior of neutrinos within localized periodic boxes of meter size, and found that the solution of the neutrino quantum kinetic equation relaxes to a quasistationary state whose properties can be modeled by simple analytical formulae subject to the conservation laws, when coarse-grained over the box size [3,6]. Furthermore, we identified later that for the solution of the global neutrino quantum kinetic transport in a realistic supernova background profile, the local coarse-grained properties of neutrinos resemble those obtained in local periodic box simulations [4]. Encouraged by these findings, we proposed a new framework that utilizes the scale separation to efficiently take into account the quantum effect of neutrino oscillations in an effective classical transport model [5]. We show that with this framework, the effective model is capable of accurately capturing the effect of flavor oscillations without resolving the tiny quantum oscillation scale, hence adding little computational burden to the existing architecture of classical neutrino transport solver used in supernova simulation (see Fig. 1). Thus, it offers a way going forward to include this missing piece of physics in supernova models. We fully expect that such an implementation can be done in the next few years to shed new lights on supernova explosion mechanism.

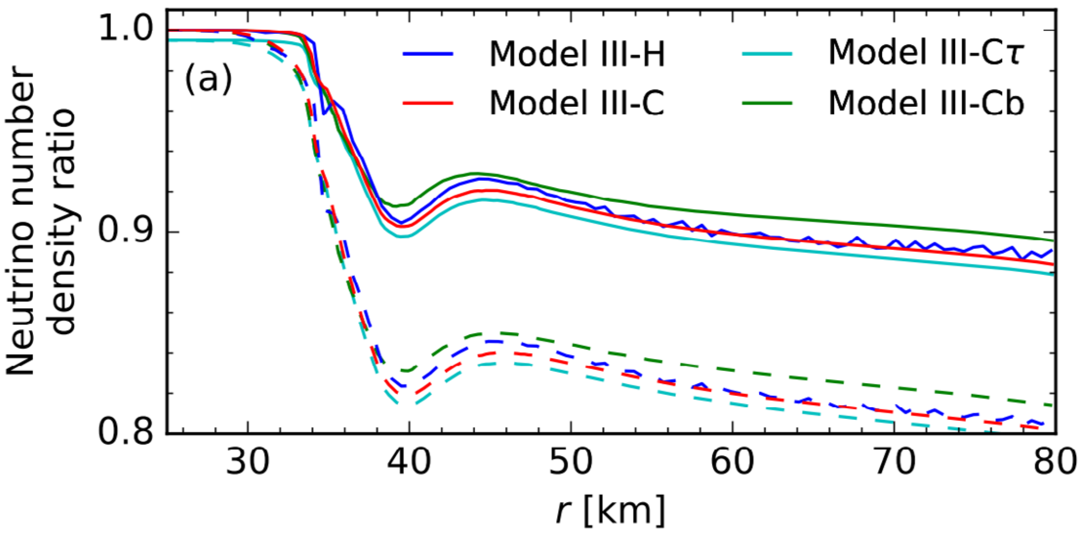


Fig. 1. The comparison of the quantum kinetic transport solution (Model III-H) with those obtained using different effective classical transport models (Model III-C, -Cτ, and -Cb) from transport simulations performed over a global supernova background profile; See [5] for details.

On another frontier, we have explored in recent years the possibility of probing the nature of dark matter by considering the scenario that they can be upscattered by the abundant amount of supernova neutrinos [7-9]. In particular, we showed that the arrival flux of the supernova-neutrino-boosted dark matter at Earth contains specific temporal shape uniquely determined by the dark matter mass and the supernova location [7]. As a results, if such a signal can be identified following the detection of supernova neutrino signals, the time-of-flight information can be used to determine the unknown dark matter mass. We have also shown that in the absence of the dark matter signals, the existing data from the large-scale neutrino experiments such as Super-Kamiokande or the projected capability of Hyper-Kamiokande can be used to place stringent and leading constraints on the interaction cross sections between the Standard Model leptons and the dark sector, by considering either the historical SN1987a event, the existence of the diffuse supernova-neutrino-boosted dark matter background, or the next Galactic supernova [8,9].

[1] T. Fischer, G. Guo, K. Langanke, G. Martinez-Pinedo, Y.-Z. Qian, M.-R. Wu, Prog. Part. Nucl. Phys. 137 (2024) 104107.
[2] M.-R. Wu, M. George, C.-Y. Lin, Z. Xiong, Phys. Rev. D 104 (2021) 10, 103003.
[3] Z. Xiong, M.-R. Wu, S. Abbar, S. Bhattacharyya, M. George, C.-Y. Lin, Phys. Rev. D 108 (2023) 6, 063003.
[4] Z. Xiong, M.-R. Wu, M. George, C.-Y. Lin,

N. K. Largani, T. Fischer, G. Martinez-Pinedo, Phys. Rev. D 109 (2024) 12, 123008.
[5] Z. Xiong, M.-R. Wu, M. George, C.-Y. Lin, arXiv:2403.17269.
[6] M. George, Z. Xiong, M.-R. Wu, C.-Y. Lin, arXiv:2409.08833.
[7] Y.-H. Lin, W.-H. Wu, M.-R. Wu, H. T.-K. Wong, Phys. Rev. Lett. 130 (2023) 11, 111002.
[8] Y.-H. Lin, T.-H. Tsai, G.-L. Lin, H. T.-K. Wong, and M.-R. Wu, Phys. Rev. D 108 (2023) 8, 083013.
[9] Y.-H. Lin, M.-R. Wu, Phys. Rev. Lett. 133 (2024) 11, 111004.

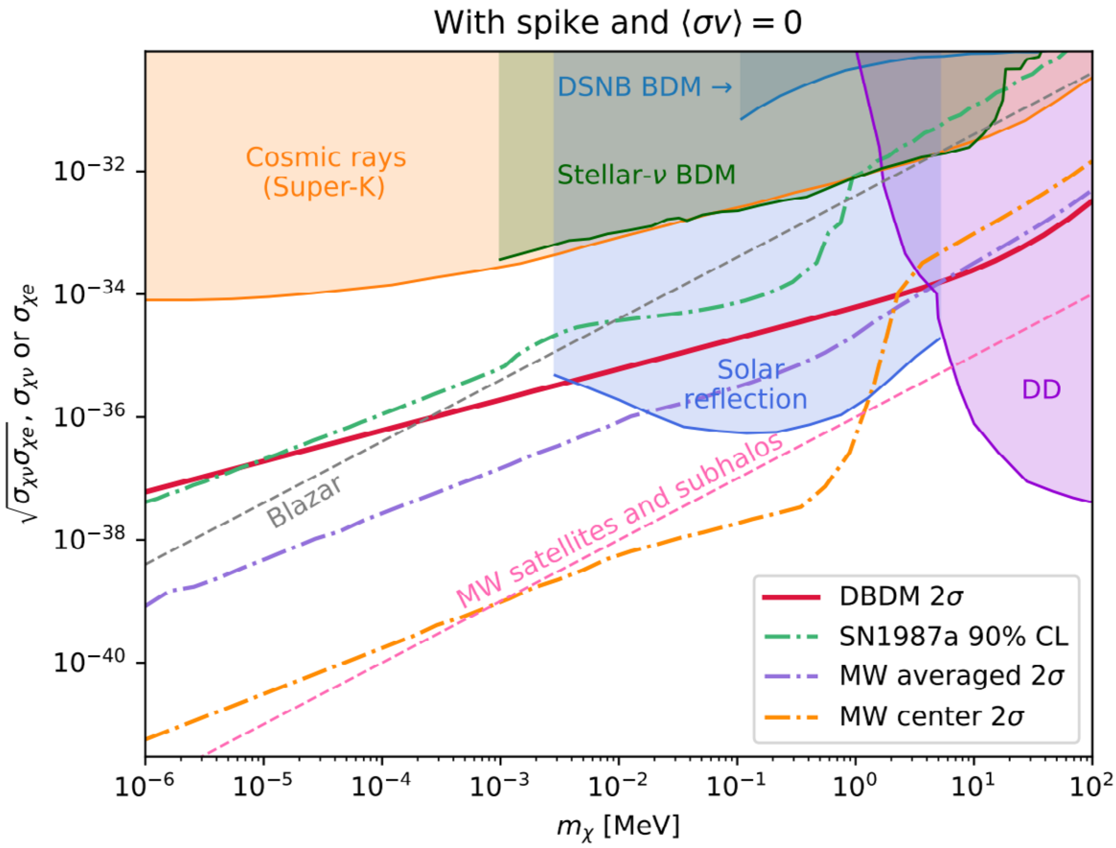


Fig. 2. The constraint from SN1987a with Super-Kamiokande data by considering the supernova-neutrino-boosted dark matter, and the projected sensitivities with Hyper-Kamiokande with the diffuse supernova-neutrino-boosted dark matter (DBDM) and with the next galactic supernova that occurs at the Milky Way (MW); see Ref. [9] for details.

Detecting Neutrinos and Dark Matter

Associate Professor

Martin Spinrath

Center Scientist

National Tsing Hua University

Particle Physics Phenomenology

In my work in recent years I have been focusing on neutrinos and dark matter. Here I want to highlight two of my articles published in 2023. In both articles we are investigating the question on how we can detect neutrinos and dark matter which were produced in the early universe.

Cosmic Neutrino Background

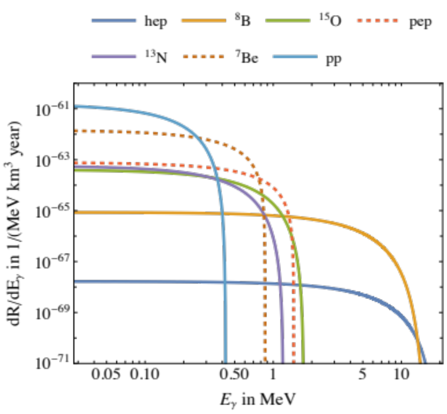


Figure 3: Event rate as a function of the energy of the emitted Bremsstrahlung photons. Taken from [1]. See details there.

A direct detection of the Cosmic Neutrino Background (CNB) has been described as a holy grail of particle cosmology due to its difficulty to achieve and promised insights into the origin of the universe. For that reason, I also got interested in it and from time to time explore an idea how it could possibly be measured in an experiment on Earth.

My paper [1] is one example for that. The challenge for the direct detection of the CNB is two-fold. First of all, due to the low-energy of the neutrinos their interaction cross section with normal matter is extraordinarily small and even if they interact with matter, the effect on matter is also very small.

In [1] we therefore explored a slightly indirect way. Suppose the CNB neutrinos scatter from any ordinary matter, then there should also be a Bremsstrahlung component with photons being emitted from that scattering process. The Bremsstrahlung photons would then have a characteristic spectrum which might be distinguished from backgrounds. For this process to happen we only have to add neutrino masses to the Standard Model of Particle Physics to generate a loop-induced magnetic dipole and/or magnetic transition moments for neutrinos. A modification which is necessary to accommodate neutrino oscillations. But there might also be other new physics contribution which enhance the dipole moment.

In [1] we therefore explored a slightly indirect way. Suppose the CNB neutrinos scatter from any ordinary matter, then there should also be a Bremsstrahlung component with photons being emitted from that scattering process. The Bremsstrahlung photons would then have a characteristic spectrum which might be distinguished from backgrounds. For this process to happen we only have to add neutrino masses to the Standard Model of Particle Physics to generate a loop-induced magnetic dipole and/or magnetic transition

moments for neutrinos. A modification which is necessary to accommodate neutrino oscillations. But there might also be other new physics contribution which enhance the dipole moment.

We then calculated neutrino-neutrino scattering Bremsstrahlung process for the first time and unfortunately it turned out that this process is very small for our chosen example where the CNB scatters from the solar neutrinos. Therefore it is unlikely that this process can be used to detect the CNB. But it might be relevant for other astrophysical and cosmological environments which we have not explored yet.

Dark Matter

Regarding Dark Matter (DM) we have also been exploring new ways to detect it on Earth.

There is overwhelming evidence for the existence of DM from different time and length scales in cosmological and astrophysical observations. But so far it remains a mystery what DM actually consists of. For decades we have put a strong experimental focus on well-motivated DM models but these searches did not find any compelling signal. For that reason, recently the attention has expanded to more exotic DM models and new experimental ideas to look for DM in other regions of the possible parameter space.
In my working group we have been interested in using quantum sensors to look for DM and in particular we have studied how Gravitational Wave (GW) detectors could be used for that purpose. They might be the biggest and most sensitive quantum sensors we have in operation which aim for a continuous operation.

In [2] we have studied how a DM object with a mass of around 10 kg could affect the movement of the pendula in KAGRA as an explicit example for a GW detector. In the presence of an additional long-range Yukawa-like interaction that could perturb the mirror motion significantly enough to produce a signal which is larger than the background noise in the detector.

In fact, with some basic common assumptions one could expect a few events of DM passing by the detector each year which is an exciting prospect. Currently, we are working on analyzing public LIGO data for such a signal and we expect to at least place one of the strongest bounds for this kind of DM which is difficult to constrain using other more conventional DM searches.

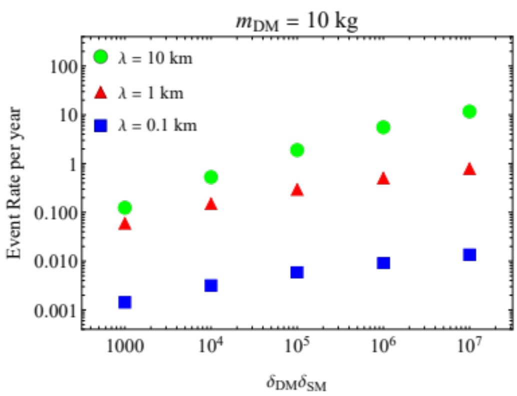


Figure 4: Estimated observable event rate for heavy DM at KAGRA using our assumptions. Taken from [2]. See more details there.

References

[1] K. Asteriadis, A. Quiroga Triviño and M. Spinrath, “Bremsstrahlung from neutrino scattering via magnetic dipole moments,” Int. J. Mod. Phys. A **38** (2023) 2350139, [arXiv:2208.01207 [hep-ph]]

[2] C.-H. Lee, R. Primulando and M. Spinrath, “Discovery prospects for heavy dark matter in KAGRA,” Phys. Rev. D **107** (2023) 035029, [arXiv:2208.06232 [hep-ph]].

Bootstrapping string theory EFT

Professor

Yu-tin Huang

Center Scientist

National Taiwan University

Gravity, effective field theory, string theory

Ever since the introduction of the Einstein-Hilbert Lagrangian as the action principle in deriving general relativity, it was clear that the theory must be an effective theory. Searching for the ultra-violet completion of general relativity (GR) has been a tremendously fertile field, leading to results relevant to high-energy, condensed matter, quantum computing and mathematics. The S-matrix bootstrap, provides an arena where one can frame the quest in the language of physical observable. One asks the following simple question: what is the 2 -> 2 scattering amplitude in gravity that satisfies the principle of unitarity, locality and causality?

To answer this question, one must be able to translate the constraints into analytic property of the physical observable, i.e. the four-point scattering amplitude M(s,t). Here s and t are momentum inner products between the incoming momenta, and between incoming outgoing momenta respectively. One captures the center of mass energy, while the other captures the angle with which the final state scattered in the center of mass frame. Then Causality is reflected that M(s,t) cannot grow faster than the square of s as the center of mass energy tends to infinity [1]. Unitarity is just the statement that the imaginary part of M(s,t) must be positively expanded on the partial waves. Finally since at low energies gravitational physics is well described by GR, we expect that any corrections to GR must at low energies appear in to form of higher dimensional (irrelevant) local operators, which in principle has an infinite expansion in derivatives and fields. This implies that M(s,t) has a Laurent series representation at small s, t.

Wilson coefficients	Two-sided bound	Superstring value	Relative error
$\tilde{b}_{1,0}$	$1.20203 < \tilde{b}_{1,0} < 1.202059$	1.202056	2.4×10^{-5}
$\tilde{b}_{2,0}$	$1.08231 < \tilde{b}_{2,0} < 1.08233$	1.082323	1.8×10^{-5}
$\tilde{b}_{3,2}$	$0.09653 < \tilde{b}_{3,2} < 0.0966$	0.09655	7.2×10^{-4}
$\tilde{c}$	$-1\times10^{-6} < \tilde{c} < 2\times10^{-5}$	0	N/A

The coefficients of the Laurent series are the Wilson coefficients of the effective field theory, and encodes the information of the ultra-violet completion. If there is a unique completion, then the Wilson coefficient will be unique. Thus for example, if string theory is the unique theory of quantum gravity, then one should be able to show that the allowed region of these Wilson coefficients are spanned by that derived from string theory. Indeed we have seen some promising result in [2,3]. For example by assuming 10 dimensional maximal supersymmetry, in [2] it was shown that allowed region of Wilson coefficient for the R^4 operator is exactly spanned by Type-II A and B string theory values.

In collaboration with my students, we pose the question in the other direction [4]. That is, what is the space of EFT's spanned by the presence of a worldsheet? In other words, can one at least prove that the current known string theories are the unique theory describing a string propagating in flat background. We study the space of open string effective field theories by combining the constraint of unitarity and monodromy relations for the four-point amplitude. The latter is a refection of an underlying disk correlator with singularities at the boundary. By assuming maximal susy the resulting bootstrap isolates Wilson coefficients to at least 10−4 of the Type-I superstring. For example for the Wilson coefficients of D^2F^4, D^4F^4, D^8F^4.

D	$\tilde{g}_{k,q}$	Two-sided bound	Superstring value	Relative error
4	$\tilde{g}_{1,0}$	$1.20204774 < \tilde{g}_{1,0} < 1.20205755$	1.20205690	8.1×10^{-6}
4	$\tilde{g}_{3,0}$	$1.03692704 < \tilde{g}_{3,0} < 1.03692956$	1.03692775	2.4×10^{-6}
4	$\tilde{g}_{4,1}$	$0.0405367063 < \tilde{g}_{4,1} < 0.0405469176$	0.0405368972	2.5×10^{-4}
10	$\tilde{g}_{1,0}$	$1.20205185 < \tilde{g}_{1,0} < 1.20205700$	1.20205690	4.3×10^{-6}
10	$\tilde{g}_{3,0}$	$1.03692764 < \tilde{g}_{3,0} < 1.03692814$	1.03692775	4.8×10^{-7}
10	$\tilde{g}_{4,1}$	$0.0405368583 < \tilde{g}_{4,1} < 0.0405426553$	0.0405368972	1.4×10^{-4}

Furthermore, utilizing our geometric approach to the bootstrap program developed in [5], we obtain the critical dimension of 10 from the low energy coefficients alone. Remarkably, relaxing SUSY but requiring the massless states to carry four-dimensional helicities, the Wilson coefficients are again constrained to superstring values within 10−4 . For example the coefficients for D^2F^4, D^4 F^4, D^6 F^4 and F^3 is fixed to. Thus we conclude that ***type-I string theory is the unique solution to the monodromy bootstrap with either maximal susy or vector external states***. We also introduce Tachyons to the bootstrap and demonstrate for the scattering of external vectors, the bosonic and superstring span the allowed region. Allowed regions for closed string efective feld theories are obtained by implementing the KLT relations.

1. ``Gravitational Regge bounds,'' K. Haring and A. Zhiboedov, SciPost Phys. 16, no.1, 034 (2024)
2.``Where Is String Theory in the Space of Scattering Amplitudes?,'' A.~Guerrieri, J. Penedones and P. Vieira, Phys. Rev. Lett. 127, no.8, 081601 (2021)
3. ``Where is tree-level string theory?,'' J. Albert, W. Knop and L. Rastelli, arXiv:2406.12959
4. ``Bootstrapping string theory EFT,'' L. Y. Chiang, Y. t.Huang and H. C. Weng, JHEP 05, 289 (2024)
5. ``Into the EFThedron and UV constraints from IR consistency,'' L. Y. Chiang, Y. t. Huang, W. Li, L. Rodina and H. C. Weng, JHEP 03, 063 (2022).

Proposal for Quantum Gravity and quantum mechanics of black hole

Professor

Chong-Sun Chu

Center Scientist

National Tsing Hua University

Quantum Field Theory, String Theory and Gravity

Entanglement and Holography

In 2017, I have made a new proposal for the holographic duality for Boundary Confornal Field Theory (BCFT) with conformal boundary condition (CBC) [1,2]. Stronger motivation to study CBC was later provided by Witten who showed that CBC of gravity is elliptic and hence always leads to well-defined perturbation theory of gravity. Traditionally, entanglement refers to the quantum correlation between subsystems defined at an equal time slice. Recently the concept of time-like entanglement entropy was introduced as a mean to describe quantum correlation between subsystems that are defined at equal space, in which case presumably the correlation between different parts of quantum histories is being studied. In my recent work [1], we discovered a novel phase of timelike entanglement entropy in BCFT that is associated with the Regge singularity. Our work on AdS/BCFT has injected new energy to this subject of research originally initiated by Takayanagi in 2011 and have in the development of the island proposal for resolution of the entanglement entropy for Hawking radiation. Scaling symmetry plus Lorentz symmetry in a field theory implies conformal symmetry. This is not the case in non-relativistic theory, e.g. anisotropic theory. Recently, we have succeeded in constructing Lifshitz field theory which has an arbitrary index z of anisotropy [2]. Lifshitz scale invariance is interesting as it describes the quantum critical point of non-relativistic systems. In [3], we put forward a new holography duality for boundary Lifshitz Field Theory (BLFT). Our work is leading and opening up new avenue of research.

[1] Chong-Sun Chu, Himanshu Parihar, Time-like entanglement entropy in AdS/BCFT,JHEP 06 (2023) 173

[2] J. Basak, A. Chakraborty, C.S. Chu, D. Giataganas,H. Parihar, Massless Lifshitz field theory for arbitrary z, JHEP 05 (2024) 284

[3] Chong-Sun Chu Himanshu Parihar, Holography for Boundary Lifshitz Field Theory, 2409.06667 [hep-th]

Quantum Mechanics for Quantum Gravity and Black Holes

There are mounting theoretical evidences that black hole has an entropy and a temperature due to a thermal Hawking radiation. Yet, it is not known what quantum gravitational degrees of freedom makes up the entropy. In [4], a novel fermionic quantum vacuum of black hole was proposed. Previously, both in matrix theory or string theory construction of black hole, the vacuum is always bosonic. Our work points out the possibility of a degeneracy pressure that is able to sustain the gravitational collapse and present the formation of a singularity inside the black hole. The idea is further elaborated in [5] where we show that Schwarzschild horizon radius is reproduced and the counting of these fermi microstates reproduces precisely the Bekenstein-Hawking entropy. In [6], we include the effect of tunneling and reproduces the Page curve of Hawking radiation. We also show that the entirety of information initially stored in the black hole is returned to the outside via the Hawking radiation. In this summer 2024, a quantum mechanical theory of quantum spaces described by a large N non-commutative coordinates is proposed as a theory for quantum gravity [7]. The theory admits as static solution fuzzy sphere whose mass-radius relation agrees exactly as that of a Schwarzschild black hole. Moreover, it has a sets of microstates whose counting reproduces exactly the Berkenstein-Hawking entropy of black hole. The proposal was further justified by the fact that the Kerr black hole is also described in our theory. It was shown in [8] that the theory has a rotating non-commutative geometry as a solution. Due to rotation, the fuzzy sphere is deformed into a fuzzy ellipsoid, which matches exactly the outer horizon of the Kerr black hole in the Boyer-Lindquist coordinates. Furthermore the fuzzy solution reproduces the Bekenstein-Hawking entropy as well as the mass of the Kerr black hole. These results provide further support that our proposed theory of quantum spaces is a plausible candidate for the theory of quantum gravity.

[4] Chong-Sun Chu, Rong-Xin Miao, Tunneling of Bell Particles, Page Curve and Black Hole Information, e-Print: 2209.03610 [hep-th]

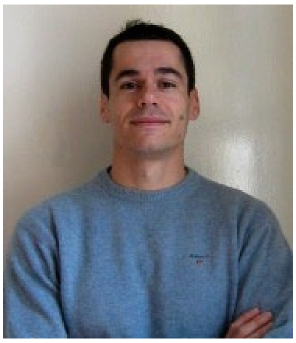
[5] Chong-Sun Chu, Rong-Xin Miao,A Fermi Model of Quantum Black Hole, Phys.Rev.D 110 (2024) 4, 046001

[6] Chong-Sun Chu, R-X Miao, Tunneling, Page Curve and Black Hole Information, e-Print: 2307.06176 [hep-th]

[7] Chong-Sun Chu, A Matrix Model Proposal for Quantum Gravity and the Quantum Mechanics of Black Holes, 2406.01466 [hep-th]

[8] Chong-Sun Chu, Quantum Kerr Black Hole from Matrix Theory of Quantum Gravity, 2406.12704 [hep-th]

Quasinormal Modes, Universality and Holography of the Penrose Limit of Black Hole Photon Rings



Assistant Professor

Dimitrios Giataganas

Center Scientist

National Sun Yat-sen University

High energy theory

All black holes possess an event horizon, the area of which is linked to the black hole's entropy, naturally corresponding to the number of all possible microstates of the black hole. A central question then arises: where do these microstates reside in the quantum dual description? The most natural hypothesis is that this information lies on the event horizon or within a few Planck lengths of it. Additionally, all black holes feature bound null geodesics, known as the photon ring which is located far from the event horizon, and can now be observed through black hole imaging, while with future space-based very-long-baseline interferometry, we will obtain even more precise data [1]. These unstable null geodesics produce the observable photon ring, which turns out to encode crucial insights of black hole properties. Any object falling into the black hole must cross the photon shell before reaching the event horizon, thereby exciting photons within the photon ring of an asymptotically flat black hole. These excited photons eventually escape after orbiting the ring multiple times, representing the last detectable signal after the black hole returns to its ground state due to this infall-induced excitation. There lies the relationship between quasinormal modes in the geometric optics approximation and lightlike geodesics. Beyond being a fundamental probe of black holes, this description suggests that the photon ring qualifies as part of the holographic dual, at least for asymptotically flat black holes [2,3]. Consequently, in-depth studies of black hole photon rings offer a compelling field within gravitational physics, spanning observational physics and quantum black hole theory. A significant advancement in these studies would be developing a generic framework based on black holes' general characteristics and symmetries, readily applicable across diverse, interesting spacetimes. This approach is promising since the way that the connection of the black hole with its photon ring properties is established, remains largely independent of the very specific black hole details.

Working in this direction we have examined the geometry observed by an observer traveling near light speed around the photon ring, known as the Penrose limit, which depends on the black hole's properties [2]. Our findings show that the Penrose limit encodes essential black hole information. Specifically, the black hole's return to equilibrium after excitation is directly encoded in the Penrose limit of the photon ring, located far from the event horizon. More technically, solutions to the massless scalar wave equation in the black hole background, particularly the quasinormal modes, correspond to the instability of the photon ring's null geodesics. Thus, the

Lyapunov coefficients of these null geodesics and the quasinormal modes relate directly to the plane wave geometry Hamiltonian, meaning that knowledge of the Penrose limit's plane wave geometry reveals everything about the quasinormal modes and the Lyapunov exponents of the photon ring's null geodesics, by a simple exciting, universal relation.

This naturally raises the question of whether the photon ring is part of holographic duality. We have found that the out-of-time-order correlator of a dual thermal quantum field theory, with a maximally chaotic Lyapunov exponent matching that of the unstable geodesics of the photon ring, emerges when the dual theory's temperature T equals the Unruh temperature of the photon ring, viewed as an effective Rindler horizon [2]. This is a direct signal relating the photon ring to the holography of asymptotically flat black holes. Moreover, we predict a maximal Lyapunov exponent complying with a chaos bound set by the inverse square root of the theory's entropy. Our findings and the framework is universal, applying to various spacetimes, including stationary black holes (e.g. Kerr, Kerr-Newman) and static black holes (e.g., Schwarzschild, Reissner–Nordström), among many others.

[1] Observing the Inner Shadow of a Black Hole: A Direct View of the Event Horizon, Andrew Chael, Michael D. Johnson, Alexandru Lupsasca
e-Print: 2106.00683 [astro-ph.HE],
Astrophys.J. 918 (2021) 1, 6
[2] Quasinormal modes and universality of the Penrose limit of black hole photon rings, D. Giataganas, A. Kehagias, A. Riotto, e-Print: 2403.10605 [gr-qc],
DOI : 10.1007/JHEP09(2024)168
[3] Holography of the photon ring, S. Hadar, D. Kapec, A. Lupsasca, and A. Strominger, Class.Quant. Grav. 39, 215001 (2022), arXiv:2205.05064 [gr-qc]

New flavors of the streaming instability in planet formation

Associate Research Fellow

Min-Kai Lin

Center Scientist

Academia Sinica

Planet formation and evolution

Conventional planet formation theory begins with small, micron-sized dust grains embedded in gaseous protoplanetary disks (PPDs) orbiting young stars. Upon collisions, these micron-sized dust particles stick together through surface forces, allowing them to grow. Collisional growth is effective until dust reaches mm-cm sizes, which is called pebbles in this context. Beyond pebbles, however, growth is threatened by fragmentation or bouncing upon collisions. Furthermore, drag forces from the gas tend to cause pebbles to drift rapidly to the star and are quickly lost from the system.

However, suppose a cloud of pebbles forms with a high mass density. In that case, its collective self-gravity can drive a direct collapse into planetesimals—km or larger-sized bodies that can proceed to build planets. This bypasses intermediate scales, which are most vulnerable to fragmentation and drift. Many theoretical efforts have, therefore, been devoted to identifying and modeling mechanisms to form dense pebble clouds in PPDs.

Over the last two decades, the ‘streaming instability’ (SI, Youdin & Goodman, 2005; Youdin & Johansen, 2007) has emerged as a promising route to concentrate pebbles to the required densities for gravitational collapse. The SI is a generic instability in rotating dust and gas mixtures, which is precisely what PPDs are made of. However, in reality, PPDs are complex objects involving a plethora of other physical effects. It is, therefore, critical to assess the viability of the SI as a planetesimal formation mechanism under realistic conditions expected in PPDs.

Our team has developed theoretical and computational models of the SI to account for various effects, including turbulence, disk structure, thermodynamics, and, recently, accretion flows and magnetic fields. We often find the classical SI is weakened. Still, we have also identified novel variations of the instability that could facilitate planetesimal formation in situations where the classical SI is ineffective. We highlight results from our latest discoveries below. PPDs are fundamentally accretion disks: material slowly drains onto the central star. The current consensus is large-scale magnetic fields mediate the accretion. We previously discovered a new ‘azimuthal drift SI’ (AdSI) in disks that exhibit gas accretion (Lin & Hsu, 2022; Hsu & Lin, 2022). We extended these first studies to an extensive parameter survey using high-resolution, state-of-the-art computer simulations (Wang & Lin, in press). Fig. 1 shows selected simulations for different initial values of the dust-to-gas mass ratio, ε. The AdSI readily forms filaments, even for ε less than unity. This contrasts with the classical SI, which typically requires ε > 1 to produce clumping. Furthermore, we showed that an accretion flow can promote filament formation when the classical SI dominates a system but cannot form filaments on its own.

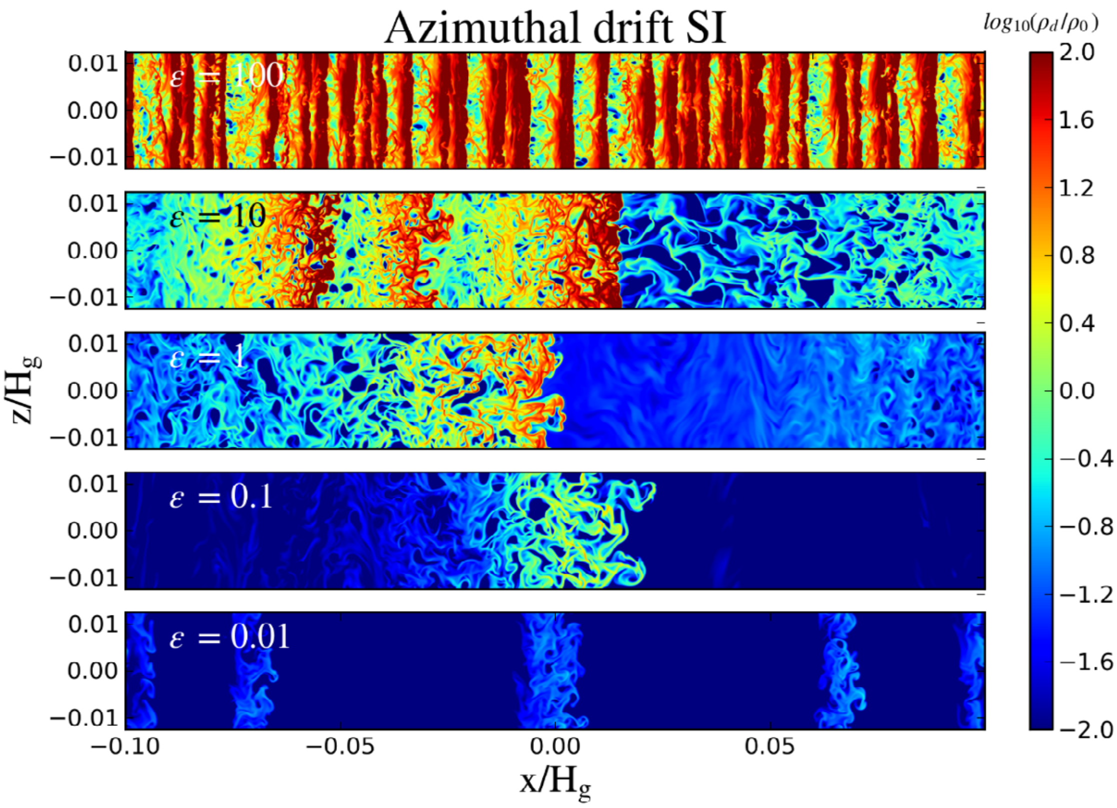


Fig. 1 — Numerical simulations of the ‘azimuthal drift streaming instability’ for different initial values of the dust-to-gas mass ratio (ε), from 100 to 0.01 (top to bottom). The final dust density distribution is shown on a logarithmic scale.

Magnetic fields can drive small-scale gas instabilities in addition to large-scale accretion. However, despite the importance of both effects in PPDs and planetesimal formation, the impact of magnetic fields on dust dynamics (and vice versa) has seldom been studied. To this end, we analyzed the stability of dusty, magnetized gas, accounting for the Hall effect (Wu et al., 2024), which is considered relevant in planet-forming regions of PPDs.

We discovered a magnetic instability triggered by the gas drift induced by dust. This ‘Background Drift Hall Instability’ (BDHI) can dominate weakly magnetized, dust-poor systems. The left panel of Fig. 2 shows a numerical simulation of the BDHI compared to the classical SI in the right panel. As can be seen, the classical SI produces large-scale but gentle fluctuations, whereas the BDHI produces small-scale, more intense variations in the dust densities with larger amplitudes. The BDHI may thus be relevant and possibly provide an alternative route to planetesimal formation in dust-poor regions of PPDs. This work was led by a PhD student at the University of Leicester (UK) and in collaboration with one of our TG’s core members.

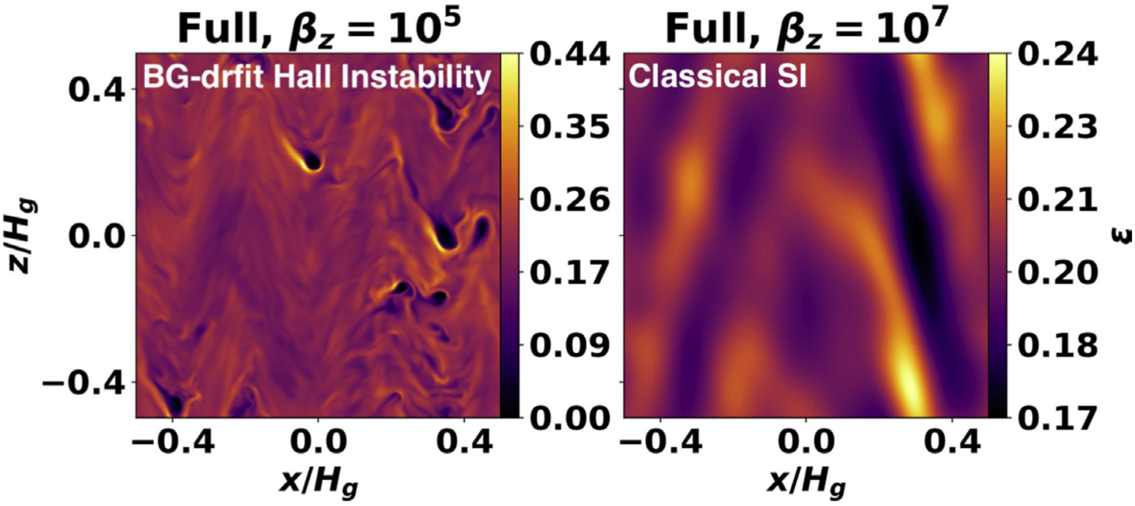


Fig. 2 — Left: Numerical simulations of a dusty, magnetized gas exhibiting the newly identified Background drift Hall instability. Right: The same simulation with negligible magnetic fields showcases classical SI. The dust-to-gas density ratio is shown.

References

Lin, M.-K., Hsu, C.-Y., 2022, ApJ, 926, 14
Hsu, C.-U., Lin, M.-K., 2022, 937, 55
Wang, S.-C., Lin, M.-K., ApJ, in press
Wu, Y., Lin, M.-K., Cui, C., Krapp, L., Lee, Y.-N., Youdin, A.N., 2024, ApJ, 962, 173
Youdin, A. N., Goodman, J., 2005, ApJ, 620, 459
Youdin, A.N., Johansen, A., 2007, ApJ, 662, 613

Scrutinizing Fuzzy Dark Matter

Associate Professor

Hsi-Yu Schive

Center Scientist

National Taiwan University

Computational Astrophysics

Fuzzy Dark Matter (FDM) is one of the leading dark matter candidates. Composed of ultralight bosons with a particle mass of $m \sim 10^{-22} - 10^{-19}$ eV, FDM exhibits distinctive wave-like properties, such as compact soliton cores and granular halos. Our research focuses on developing advanced FDM simulations to compare with various astrophysical observations, including two-component FDM models, galactic disk heating, strong gravitational lensing, and cosmological zoom-in simulations.

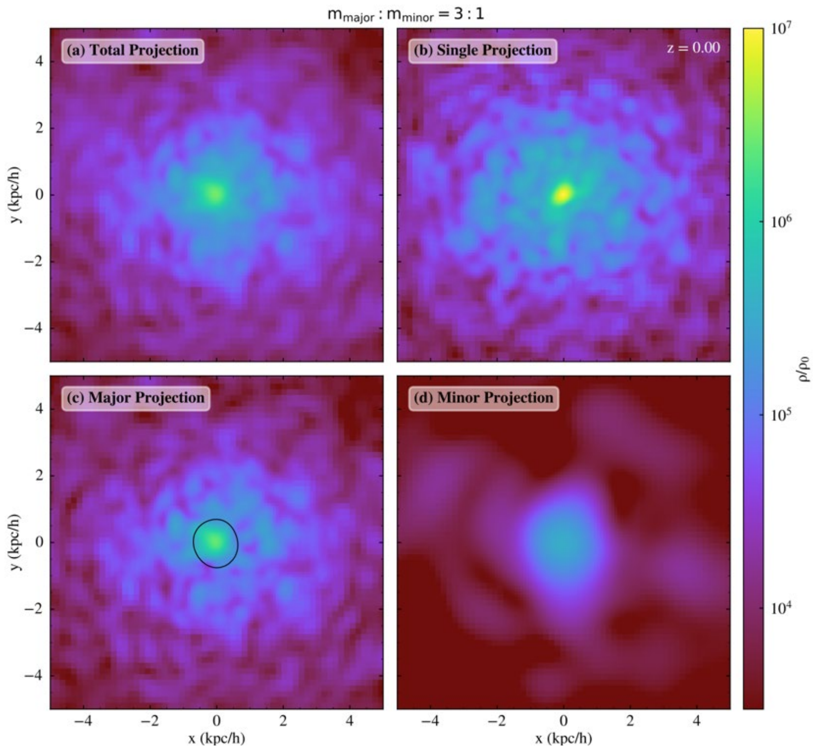


Fig. 1. Two-component FDM halo (a, c, d) with m_{major} / m_{minor} = 3 and its single-component counterpart (b). The major- and minor-component solitons coexist and are approximately concentric.

- **Two-component FDM**

In Huang et al. (2023) [1], we conducted pioneering FDM cosmological simulations that extended the traditional single-component model to two components with distinct particle masses, m_{major} and m_{minor}, coupled by gravity. Our simulations examine the soliton-halo structure in two configurations, m_{major}:m_{minor} = 3:1 and 1:3. For the 3:1 configuration, our findings reveal that (i) the major- and minor-component solitons coexist, possess comparable masses, and are approximately concentric (see Fig. 1). (ii) The soliton peak density is significantly lower than in the single-component case, resulting in a smoother rotation curve that may alleviate observational tensions associated with the single-component model.

In dramatic contrast, for the 1:3 configuration, a stable minor-component soliton cannot form when a major-component soliton is present. Consequently, the total density profile, encompassing both halo and soliton, is dominated by the major component and closely resembles the single-component scenario.

- **Galactic disk heating**

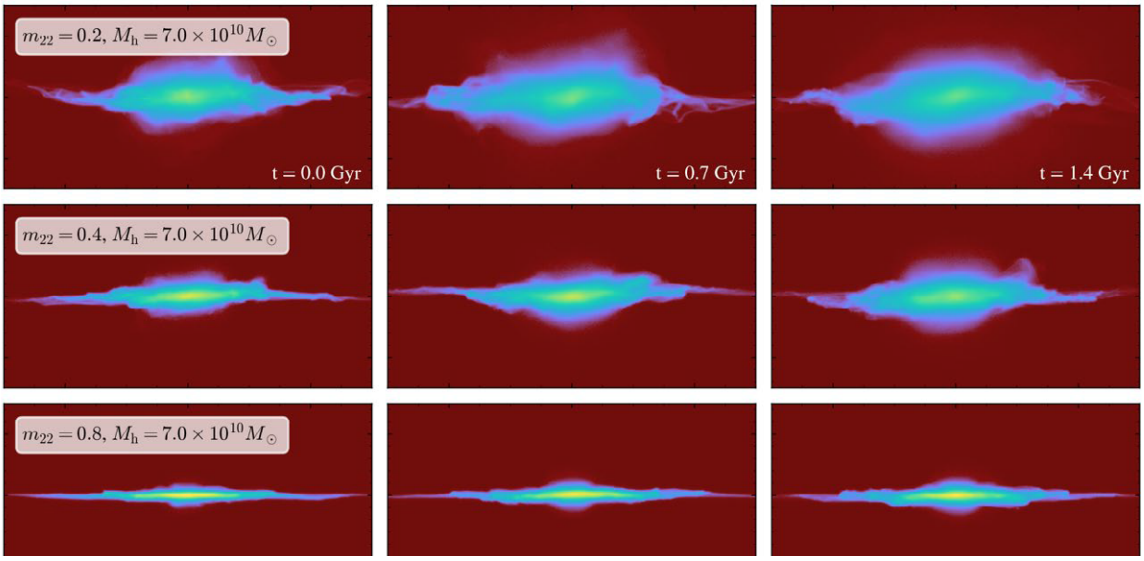


Fig. 2. Thickening of stellar disks caused by heating from FDM granule oscillations. Smaller FDM particle masses (m_{22}) result in stronger heating and, consequently, thicker stellar disks.

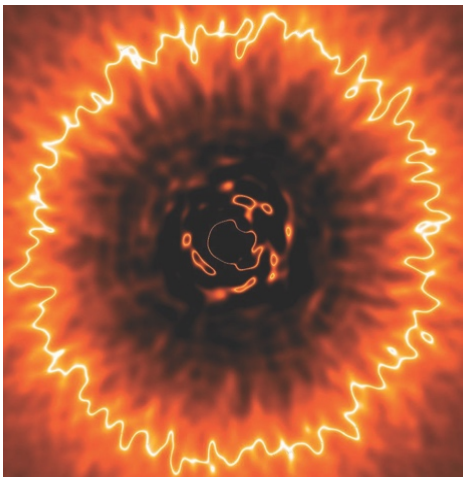


Fig. 3. Gravitational lensing in FDM.

- **Strong gravitational lensing**

The quantum interference in FDM manifests as wave patterns. An international team, including the NTU group, demonstrated that gravitational lensing in FDM leaves distinctive signatures in multiply lensed images of background galaxies (see Fig. 3), which accurately predict the level of flux anomalies that challenges the conventional cold dark matter lens models. This work is featured as the cover story in *Nature Astronomy* [4].

In Yang et al. (2024) [2], we conducted the first self-consistent simulations of stellar disks embedded within granular FDM halos to investigate disk thickening driven by the stochastic density fluctuations from quantum wave interference. We observe disk thickening across all simulated systems (see Fig. 2), with heating rates that remain approximately constant over time and increase significantly as the FDM particle mass, m_{22} (normalized to 10^{-22} eV), decreases. For m_{22} = 1.2 (0.2) and a halo mass of M_h = 7×10^{10} $M_\odot$, we measure heating rates of dh/dt ~0.04 (0.4) kpc/Gyr and $d\sigma_z^2/dt$ ~ 4 (150) $km^2/s^2/Gyr$, where h is the disc scale height and σ_z denotes the stellar vertical velocity dispersion. These simulated heating rates align within a factor of two with the theoretical predictions from Chiang et al. (2023) [3], confirming that the rough estimates by Church et al. (2019) overestimate the heating effects by two orders of magnitude.

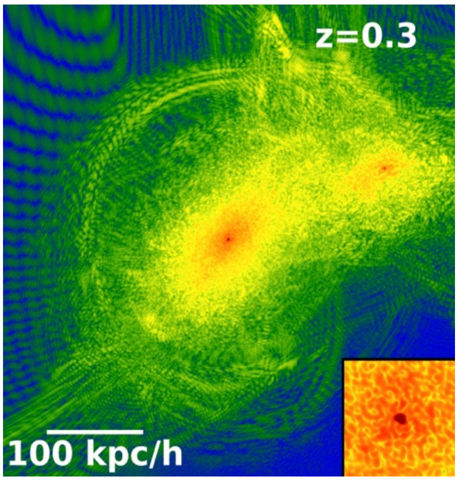


Fig. 4. FDM cosmological zoom-in simulation for a Milky Way-sized halo with a subhalo being accreted at z = 0.3. The subplot zooms into the central soliton of the host halo.

- **Cosmological zoom-in simulations**

In collaboration with Dr. Jowett Chan, an NCTS postdoctoral researcher, we conducted an FDM cosmological zoom-in simulation with m_{22} = 0.2 to evolve a Milky Way-sized halo, including its substructures, from redshift z=100 to the present day (see Fig. 4). Using a newly developed fluid-wave hybrid algorithm, this simulation allows us, for the first time, to study the evolution of FDM subhalos—from isolated structures to tidally stripped remnants—through fully self-consistent interactions with the host halo. We observe tidally stripped subhalos that deviate from the core-halo mass relation and changes in density granulation size due to the tidal stripping and heating effects from the host halo.

- **References**

[1] H. Huang, *H.-Y. Schive, and T. Chiueh, Cosmological simulations of two-component wave dark matter, Mon. Not. R. Astron. Soc. 522, 515 (2023).

[2] H.-Y. Yang, B. T. Chiang, G.-M. Su, *H.-Y. Schive, T. Chiueh, and J. P. Ostriker, Galactic disc heating by density granulation in fuzzy dark matter simulations, Mon. Not. R. Astron. Soc. 530, 129 (2024).

[3] B. T. Chiang, J. P. Ostriker, and H.-Y. Schive, Can ultralight dark matter explain the age–velocity dispersion relation of the Milky Way disc: A revised and improved treatment, Mon. Not. R. Astron. Soc. 518, 4045 (2022).

[4] Amruth et al., Einstein rings modulated by wavelike dark matter from anomalies in gravitationally lensed images, Nature Astronomy 7, 736 (2023).

[5] H.-Y. J. Chan, *H.-Y Schive, V. H. Robles, A. Kunkel, G.-M. Su, and P.-Y. Liao, Cosmological zoom-in simulation of fuzzy dark matter down to *z* = 0: tidal evolution of subhaloes in a Milky Way-sized halo, Mon. Not. R. Astron. Soc., submitted (2024).

AGN Jet-inflated Bubbles as Possible Origin of Odd Radio Circles

Associate Professor

Hsiang-Yi Karen Yang

Center Scientist

National Tsing Hua University

Astrophysics

Recent cosmological simulations have demonstrated the importance of cosmic rays (CRs) in the feedback processes including supernova feedback and active galactic nucleus (AGN) feedback by supermassive black holes (SMBH). It is therefore demanded to incorporate the relevant CR physics in magnetohydrodynamic (MHD) simulations in order to investigate the roles of CRs in the various astrophysical processes in the Universe.

One enigmatic phenomenon which may be related to CR feedback is the odd radio circles (ORCs). ORCs are a new class of faint, circular radio objects discovered in 2021 [1]. By identifying potential host galaxies at the center of the ORCs, it is found that they are extragalactic in origin. Their physical sizes are estimated to be ~300-600 kpc in diameter. The surface brightness distributions tend to be limb-brightened (see right column of Figure 1). To date, counterpart emission in other wavelengths has not yet been detected, and their physical origin is currently unknown. Proposed mechanisms for ORC formation include star formation shocks, accretion shocks around galaxies, and end-on AGN jet-inflated bubbles [2]. Our work focuses on the last scenario, with the aim to investigate whether AGN bubbles viewed on-axis is a plausible mechanism for producing the key features of the observed ORCs.

In our recent publication [3], we carried out 3D CR-MHD simulations using the FLASH code for modeling the long-term evolution of AGN jet-inflated bubbles. Because the sizes of the observed ORCs are large (~300-600 kpc), it is likely produced by powerful, long duration AGN jets in low-mass galaxy clusters/groups. To this end, we performed a parameter study of varied jet power, jet duration, and mass of the cluster. We assume the jets to be CR proton (CRp) dominated, because previous studies have found that CR dominated bubbles tend to be “fatter” than thermal-energy dominated bubbles [4], and thus CRp bubbles are more likely to form large circular objects when viewed end-on. In order to produce simulated radio maps, we compute the synchrotron emission of secondary CR electrons (CRe) generated during the hadronic collisions between the CRp within the bubbles and the ambient cluster gas.

Figure 1 shows the comparison between the simulated radio images (left column) with the observed images of ORC1 and ORC5 (right column). We confirm previous conjecture that, when viewed along the axis of AGN jets, the two jet-inflated bubbles would overlap and form one circular object. For successful parameter combinations, the diameter of the simulated ORCs can reach ~300-600 kpc, similar to the observed ones. Importantly, the limb-brightened surface brightness distributions are also reproduced. This is because in our model, the radio emission comes from hadronic collisions between the CRp within the bubbles and protons in the ambient cluster medium. Since the hadronic collision rate is the highest at the surface of the bubbles, the projected radio image naturally exhibits edge-brightened intensity distribution.

In addition to reproducing the key features of the observed ORCs, we also investigated how the predictions vary with different viewing angles. Our studies found that as long as the viewing angle is aligned with the jet axis within ~30 degrees, the ellipticity of the predicted ORCs is consistent with the observed ones. This greatly relieved the requirement for perfect alignment of the AGN scenario suggested by previous works. We also made predictions for the X-ray maps observable using current and upcoming facilities. We showed that, while long exposure times (~1 Ms) are required for current X-ray telescope such as the Chandra X-ray Observatory to detect ORC counterparts, next generation mission like AXIS and Athena would be able to detect X-ray emission arising from the shocks during the bubble expansion. Our work is the first detailed study to show that the end-on AGN bubble scenario is indeed a plausible formation mechanism of the ORCs.

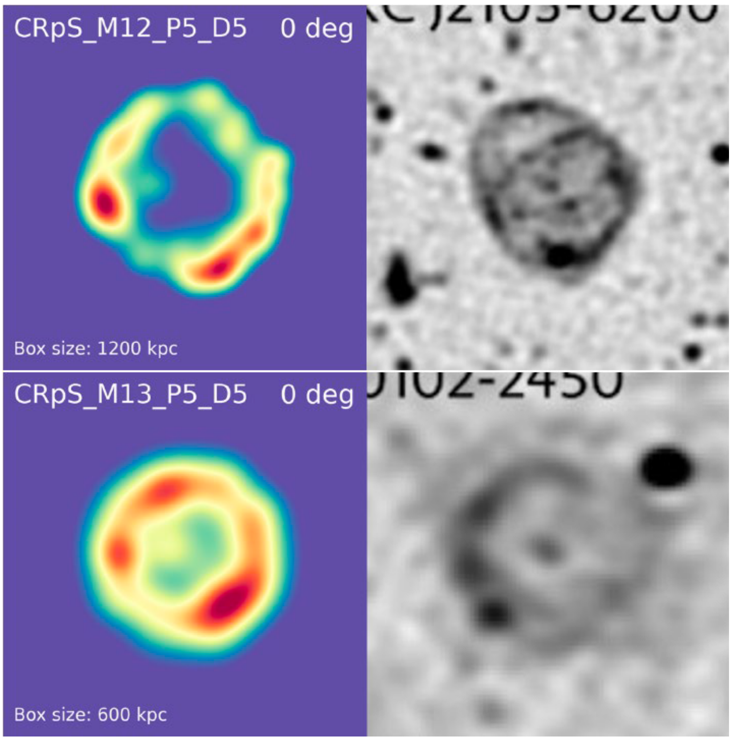


Figure 1. Representative cases of the simulated radio images (left column) compared with the observed images of ORC1 and ORC5 (right column). The sizes and limb-brightened features of the observed ORCs are well reproduced.

References:

[1] R. P. Norries, H. T. Intema, A. D. Kapinska et al., Unexpected Circular Radio Objects at High Galactic Latitude, PASA, 38, e003 [2021]

[2] R. P. Norries, J. D. Collier, R. M. Crocker et al., MeerKAT Uncovers the Physics of an Odd Radio Circle, MNRAS, 513, 1300 [2022]

[3] Y. H. Lin and H.-Y. K. Yang, AGN Jet-inflated Bubbles as Possible Origin of Odd
Radio Circles, ApJ, 974, 269 [2024]

[4] H.-Y. K. Yang, M. Gaspari and C. Marlow, The Impacts of Radio AGN Bubble Composition on the Dynamics and Thermal Balance of the Intracluster Medium, ApJ, 871, 6 [2019]

Exploring quantum materials in emergent topological phases

Professor

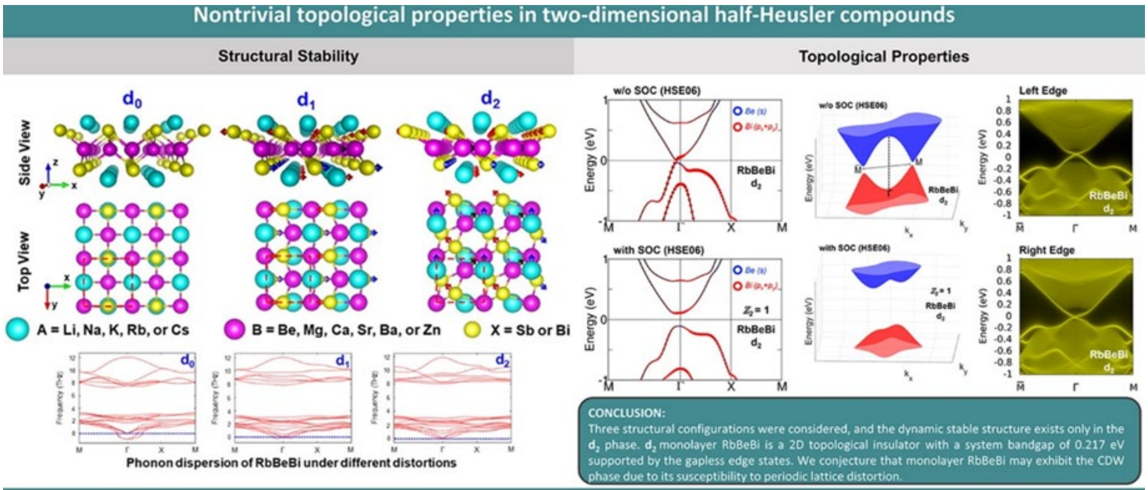
Feng-Chuan Chuang

Center Scientist

National Sun Yat-sen University

Condensed Matter Physics

The pursuit of quantum materials with exotic electronic properties has ignited a wave of research into topological phases, where materials exhibit unique characteristics governed by quantum mechanics. These emergent topological materials possess remarkable potential for next-generation technologies, from quantum computing to spintronics. In this report, several material groups that feature a rich topological landscape were explored, ranging from half-Heusler compounds to the recently synthesized MA_2Z_4 family, culminating in the discovery of higher-order topological materials.



Exploring a new frontier of two-dimensional (2D) half-Heusler compounds
With the recent synthesis of two-dimensional half-Heusler compounds, we conducted a study using high-throughput first-principles computations to explore the stability, electronic, and topological properties of 60 monolayer half-Heusler compounds with the formula ABX (A = Li, Na, K, Rb, Cs; B = Be, Mg, Ca, Sr, Ba, Zn; X = Sb, Bi) in the *P4/nmm* structure. Three structural configurations were analyzed—pristine, one-sided, and two-sided distortions. Six compounds exhibited nontrivial topological properties, with RbBeBi standing out for its largest bandgap of 0.217 eV. Orbital analysis revealed that band inversion at the Γ-point was driven by the B-element's *s*-orbital and X-element's p_x+p_y orbitals, with gapless edge states confirming a topological insulating phase. The study also speculates that monolayer RbBeBi could show charge density wave behavior due to

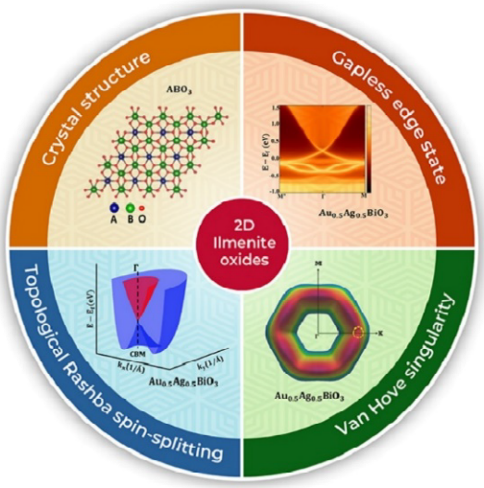
lattice distortions. This research highlights a new 2D material family, advancing the search for topological materials in future technologies.
[Chin. J. Phys. **86**, 115-121 (2023). DOI: https://doi.org/10.1016/j.cjph.2023.08.020]

Unveiling the topological and electronic wonders of 2D ilmenite oxides

This study using first-principles calculations has revealed exciting structural, electronic, and topological properties of 2D pristine ilmenite oxides, ABO_3 (A = Au, Ag, Cu; B = Bi, Sb, As), along with their Janus structures. Phonon dispersion analysis confirmed the dynamic stability of these compounds. Notably, pristine $CuBiO_3$ and $AuBiO_3$, as well as Janus structures like $Cu_{0.5}Ag_{0.5}BiO_3$, $Au_{0.5}Cu_{0.5}BiO_3$, and others, emerged as topological insulators, while some compositions such as $AuBi_{0.5}As_{0.5}O_3$ and $CuBi_{0.5}Sb_{0.5}O_3$ were identified as topological semimetals, verified by their Z_2 invariance and conducting edge states. Moreover, intriguing van Hove singularities near the Fermi level in $Au_{0.5}Ag_{0.5}BiO_3$ and $Cu_{0.5}Ag_{0.5}BiO_3$ suggest a potential coexistence of superconductivity with nontrivial topology. The study also highlighted the isotropic Rashba spin-splitting in $Au_{0.5}Ag_{0.5}BiO_3$, indicating the potential of these 2D ilmenite oxides as promising candidates for future spintronic applications.
[Chin. J. Phys. **86**, 242-254 (2023). DOI: https://doi.org/10.1016/j.cjph.2023.09.022]

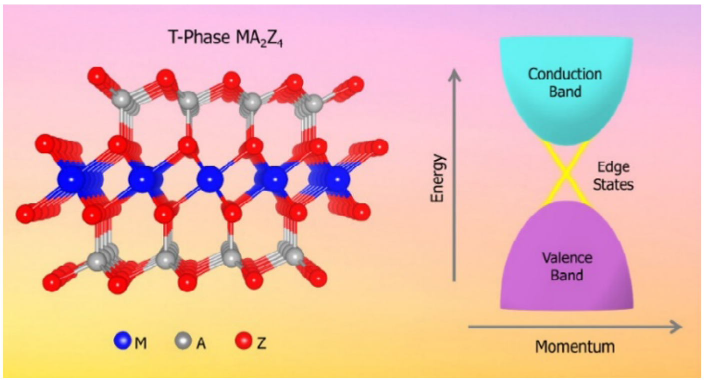
The rising star of 2D topological materials: MA_2Z_4 Compounds

A new class of two-dimensional (2D) materials known as MA_2Z_4 has captured the attention of researchers for its remarkable tunability and potential applications in electronics and topological devices. Recent theoretical studies have pushed the boundaries of what is known about the topological properties of these materials, which are defined by their flexible components: M (transition metals or alkaline earth metals), A (main group elements), and Z (pnictogens or chalcogens). In our first study, an extensive exploration of 30 MA_2Z_4 monolayers, with M = Ti, Zr, Hf, A = Si, Ge, and Z = pnictogens (N, P, As, Sb, Bi), revealed that these compounds prefer the T-phase energetically. Five of these materials—$TiSi_2Bi_4$, $ZrGe_2P_4$, $ZrGe_2As_4$, $HfSi_2As_4$, and $HfGe_2As_4$—were identified as topological insulators, driven by spin-orbit coupling (SOC). The SOC split the $\boldsymbol{d_{z^2}}$ orbitals of the transition metals and the $\boldsymbol{p_x+p_y}$ orbitals of the pnictogens, producing nontrivial band structures confirmed by Z_2 invariants and the presence of gapless edge states. Moreover, phonon spectra and ab initio molecular dynamics simulations affirmed the thermodynamic stability of these topological phases. In our second study, researchers expanded the search to MA_2Z_4 monolayers with M = Ca, Sr, Ba, A = In, Tl, and Z = chalcogens (S, Se, Te). This study uncovered quantum spin Hall (QSH) phases in $SrTl_2Te_4$ and $BaTl_2Te_4$, which displayed nontrivial bandgaps of 97 meV and 28 meV, respectively. In $SrTl_2Te_4$, the quantized spin Hall conductivity was linked to a non-zero Berry curvature, with SOC driving a band inversion

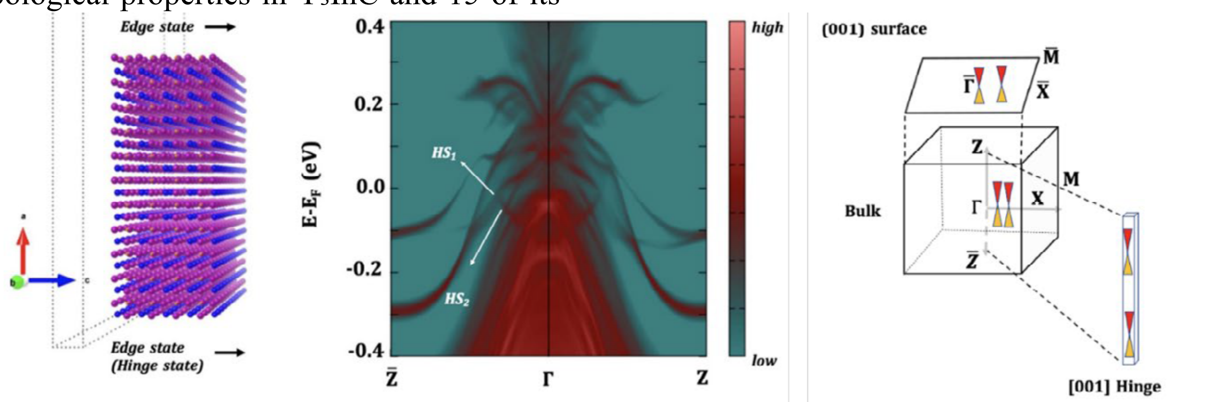


between Te-***p*** and Tl-***s*** orbitals around the Γ-point. These topological phases were found to be robust against strain and electric fields, showcasing their durability for potential device integration. Together, these studies emphasize the versatile and rich topological landscape of the MA_2Z_4 family. By unveiling both pnictogen-based and chalcogen-based topological insulators and quantum spin Hall materials, these discoveries emphasize the potential of MA_2Z_4 compounds in spintronic and topological applications, paving the way for experimental synthesis and future technological breakthroughs.
[J. Phys. Chem. **128**, 6829-6835 (2024). DOI: https://doi.org/10.1021/acs.jpcc.3c08285; Appl. Phys. Lett. **124**, 233102 (2024). DOI: https://doi.org/10.1063/5.0207576]

Exploring higher-order topological phases in Y_3InC and antiperovskite materials
Higher-order topological insulators (HOTIs), known for their unique hinge and corner states, are gaining attention for their exotic properties. However, the discovery of materials hosting both higher-order topological hinge states and gapless bulk Dirac phases has been elusive—until now. This study using first-principles calculations with hybrid exchange functionals has uncovered intriguing electronic and topological properties in Y_3InC and 15 of its related antiperovskite compounds. Without spin-orbit coupling (SOC), Y_3InC exhibits a



symmetry-protected triple point phase dominated by ***d*-*t*$_{2g}$** orbitals. When SOC is introduced, the material transitions to a twin Dirac node phase. Further analysis, including calculations of the Z_4 topological invariant, confirmed the higher-order topological nature of these materials. Remarkably, edge state calculations using a rod-shaped geometry revealed Y_3InC hosts multi-Dirac nodes in both bulk and surface phases, alongside topologically protected gapless hinge states. This groundbreaking research paves the way for future experimental and theoretical exploration of cubic antiperovskite materials as a platform for higher-order topological phases, with exciting implications for advanced electronics and quantum computing.
[New J. Phys. **26**, 073007 (2024). DOI: https://doi.org/10.1088/1367-2630/ad59ff]



Selected References

[1] Aniceto B Maghirang III, Rovi Angelo B. Villaos, Zhi-Quan Huang, Chia-Hsiu Hsu, Guoqing Chang, Feng-Chuan Chuang, Nontrivial topological properties in two-dimensional half-Heusler compounds, Chinese Journal of Physics, 86, 115 (2023).

[2] Susaiammal Arokiasamy, Gennevieve M. Macam, Rovi Angelo B. Villaos, Aniceto B. Maghirang III, Zhi-Quan Huang, Chia-Hsiu Hsu, Guoqing Chang, and Feng-Chuan Chuang, Prediction of quantum spin Hall and Rashba effects in two-dimensional ilmenite oxides, Chinese Journal of Physics, 86, 242 (2023)

[3] Ina Marie R Verzola, Rovi Angelo B. Villaos, Zhi-Quan Huang, Chia-Hsiu Hsu, Yoshinori Okada, Hsin Lin, Feng-Chuan Chuang, Nontrivial Topology in Monolayer MA_2Z_4 (M = Ti, Zr, or Hf; A = Si or Ge; and Z = N, P, As, Sb, or Bi), Journal of Physical Chemistry C 128 (16), 6829-6835 (2024).

[4] Joel D'Souza, Ina Marie R Verzola, Sreeparvathy P.C., Rovi Angelo B. Villaos, Zhi-Quan Huang, Feng-Chuan Chuang, Quantum spin Hall insulating phase in two-dimensional MA_2Z_4 materials: $SrTl_2Te_4$ and $BaTl_2Te_4$, Applied Physics Letters 124 (23), 233102 (2024).

[5] Sreeparvathy PC, Rovi Angelo B. Villaos, Zhi-Quan Huang, Feng-Chuan Chuang, Higher-order topological Dirac phase in Y_3InC: a first-principles study, New Journal of Physics 26 073007 (2024).

Electronic structures of topological semimetals and feature spectrum topology

Professor

Tay-Rong Chang

Center Scientist

National Cheng Kung University

Condensed Matter Physics

Antiferromagnetic Dirac Nodal-line semimetal

Topological semimetals with protected band crossings have garnered considerable attention in recent years. While nodal lines have been observed in some nonmagnetic materials, gapless fourfold-degenerate antiferromagnetic (AFM) nodal lines have yet to be directly detected. Simultaneously, correlated topological materials are emerging as a new frontier, where the interplay between non-trivial topology and electronic correlations can give rise to exotic phenomena such as superconductivity, fractionalization, and charge density waves. In this study, we report the discovery of an unusual gapless, fourfold-degenerate AFM Dirac nodal line in YMn_2Ge_2, based on first-principles calculations and ARPES [1]. We show that this Dirac nodal line is enforced along the boundary lines of the Brillouin zone through the interplay of magnetism, space-time inversion symmetry, and non-symmorphic mirror symmetries. These symmetries protection enables YMn_2Ge_2 to host the largest magnetic Dirac nodal line observed in any real condensed matter system to date. Furthermore, the AFM nodal line in YMn_2Ge_2 exhibits significant electronic correlation. Our findings highlight how electronic correlations influence non-trivial topology, leading to the emergence of a Hund nodal line magnet. The symmetry-enforced Dirac nodal line suggests that materials with similar magnetic or lattice symmetries could exhibit comparable correlated topological semimetallic phases.

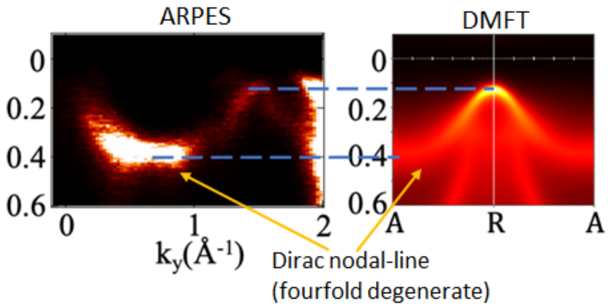


Fig.1 Band dispersion of gapless fourfold degenerate AFM Dirac nodal line.

2D Weyl semimetal

The discovery of Weyl semimetals, which host spin-split massless quasiparticles in 3D crystals, represents an exciting milestone, realizing Weyl fermions experimentally—a concept originally proposed in particle physics. Although the Weyl equation was initially derived for odd spatial dimensions, extending the 3D Weyl fermion state to 2D creates a distinct topological state of matter known as a 2D Weyl semimetal, which acts as a spin-polarized analog of graphene. This dimensional reduction gives rise to a range of unconventional physical properties, including the parity anomaly in quantum field theory, charge fractionalization with zero modes of charge e/2, spin-valley Hall effects, giant Berry curvature dipoles, and topological quantum criticality. The fascinating properties of 2D Weyl fermion states have inspired extensive theoretical and experimental exploration. In this work, we report the realization of a 2D Weyl semimetal in an epitaxial bismuthene monolayer on SnS(Se) substrates, marking the solid-state realization of Weyl fermions in 2D space [2]. The two spin-polarized valleys in this system correspond to two Weyl fermions with opposite helicities. Our demonstration of the 2D Weyl semimetal and its Fermi string edge states opens new pathways for exploring the intriguing topological quantum properties of Weyl fermions in reduced dimensions.

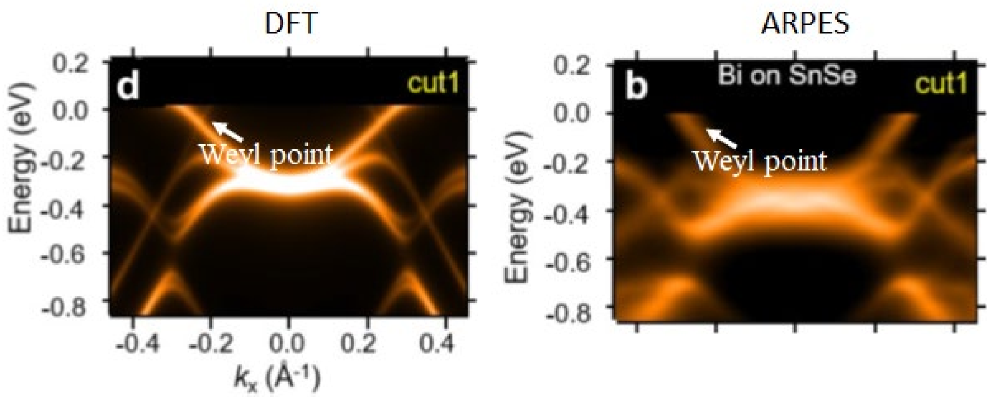


Fig.2 Band structures of the 2D Weyl semimetal.

Feature spectrum topology

Topological materials are characterized by the topological invariant numbers of electron wave functions in insulators. The bulk-boundary correspondence ensures the presence of gapless boundary states, which connect the bulk valence and conduction bands at the material's boundary when the topological invariant is an integer. In a quantum spin Hall insulator (QSHI), the topological phase is protected by time-reversal symmetry. However, symmetry-breaking perturbations, such as the Zeeman exchange field, can gap these boundary states, leading to their loss. Conventional topological band theory typically interprets this gapped phase as an ordinary band insulator. To investigate the robustness of bulk-boundary correspondence in QSHI, we apply the feature-spectrum topology approach [3]. Despite the inclusion of a symmetry-breaking term in the Hamiltonian, the feature Chern number, based on the eigenstates of each spin sector in the feature spectrum, can still be determined. Our calculations yield a feature Chern number $C_s = 1$, indicating a topologically nontrivial state. Moreover, we observe nontrivial edge states within the bulk feature eigenvalue gap, where the edge state connects the spin-up and spin-down sectors in the feature subspace. This phenomenon, which involves opening/closing of the gap in the topological edge state in the band structure, corresponds to the closing/opening in the feature spectrum, termed the feature-energy duality.

Quantum Anomalous Hall Effect in Graphene/MnBi2Te4 Heterostructure

Introduced by 2016 Nobel Prize Winner Prof. F. D. M. Haldane in 1988, the Quantum Anomalous Hall Effect (QAHE) proposes a quantized Hall conductivity in the graphene lattice, even in the absence of an external magnetic field. Despite successful QAHE realization in 3D topological insulators, achieving the QAHE in the original Haldane model within 2D graphene remains challenging. Searching the QAHE in 2D material, particularly with simplified fabrication methods, stands as a pivotal objective in modern condensed matter physics and material sciences. In this work, we propose the QAH effect in graphene/$MnBi_2Te_4$ heterostructure based on first-principles calculations [4]. Our effective Hamiltonian presents a comprehensive topological phase diagram that has not been explored previously. Taking advantage of the well-established experimental benefits offered by the graphene/Bi_2Te_3 system, coupled with the noteworthy similarity in interface structure between graphene/Bi_2Te_3 and graphene/$MnBi_2Te_4$, we assert with confidence that the experimental realization of the graphene/$MnBi_2Te_4$ heterostructure aligns with our predictions.

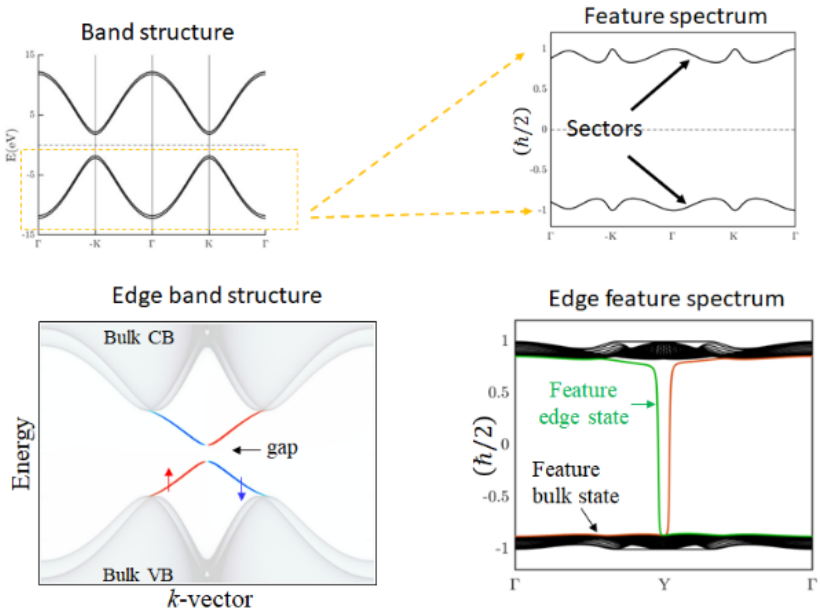


Fig.3 The bulk states and the edge states of the band structures and feature spectrum.

References

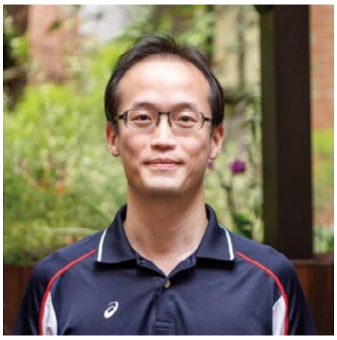
[1] Xian P. Yang et al., A topological Hund nodal line antiferromagnet, Nat. Commun. **15**, 7052 (2024).

[2] Qiangsheng Lu et al., Realization of a two-dimensional Weyl semimetal and topological Fermi strings, Nat. Commun. **15**, 6001 (2024).

[3] Yueh-Ting Yao et al., Feature-energy duality of topological boundary states in a multilayer quantum spin Hall insulator, Phys. Rev. B **109**, 155143 (2024).

[4] Y.-T. Yao et al., Atomic scale quantum anomalous hall effect in monolayer graphene/$MnBi_2Te_4$ heterostructure, Materials Horizons **11**, 3420 (2024).

Excitonic effects in two-dimensional materials



Assistant Research Associate

Yang-Hao Chan

Center Scientist

Institute of Atomic and Molecular Sciences, Academia Sinica

Computational material sciences

Excitonic effects on second order optical responses

Excitons are bound electron-hole pairs, which dominates the light absorption features of semiconductors [1]. In low dimensional system due to the quantum confinement and reduced screening effects, excitons can have large binding energy. Understanding their properties is therefore crucial for optoelectronic and photovoltaic devices applications.

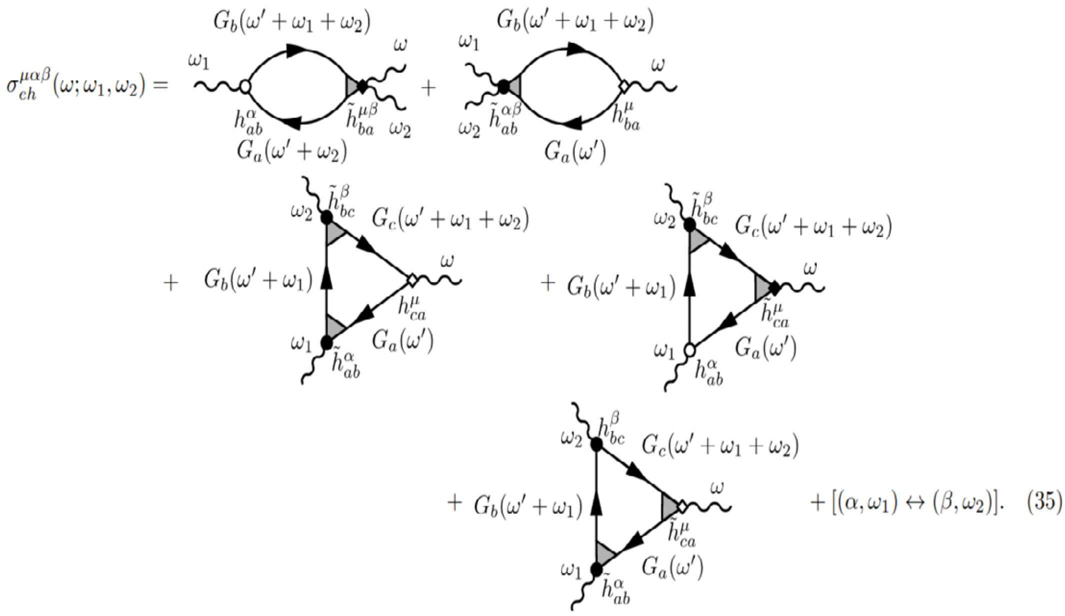


Figure 5: Diagrams for the second order optical conductivity tensor, where straight lines represent electron propagators, wiggly lines are photons, and shaded triangles are dressed vertices including excitonic effects. Figure is adopted from PRB 109, 155437.

Second order optical responses, including shift current, second harmonic generations (SHG), sum-frequency generations, and spontaneous parametric down conversion, etc., are commonly observed in noncentrosymmetric materials [2,3]. We applied a diagrammatic approach to derive a general expression for second order optical responses with excitonic effects [4]. In Fig. 1, we show the diagrams for second order conductivity tensor. The essential idea is to use the dressed vertices which include the excitonic effects. The new method is computationally much more efficient than the real-time simulation approaches we used before [5]. More importantly, it allows us to analyze inter-exciton coupling matrix elements and provides a theoretical understanding of the excitonic enhancement or the lack of it observed in the SHG spectrum for some materials. Working with Prof. Guang-Yu Guo's group in NTU, we have applied this approach to study shift current in BN nanotubes [6]. We also collaborated with the experimental group in RIKEN to understand the excitonic shift current in bulk CuI. In Fig. 2 we show the results of our recent work, we observe that the A-exciton peak in h-BN shows strong enhancement in SHG spectrum while the A-exciton peak intensity is barely seen in MoS_2 even though the two materials belong to the same space group. Our further analysis shows that the crucial difference lies in the inter-exciton coupling matrix elements in monolayer h-BN and MoS_2 [7]. In monolayer h-BN, 1s and 2p excitons are strongly coupled and both have large oscillator strength. In contrast, 2p like state in MoS_2 are dark and there is no nearby bright states for inter-exciton transitions

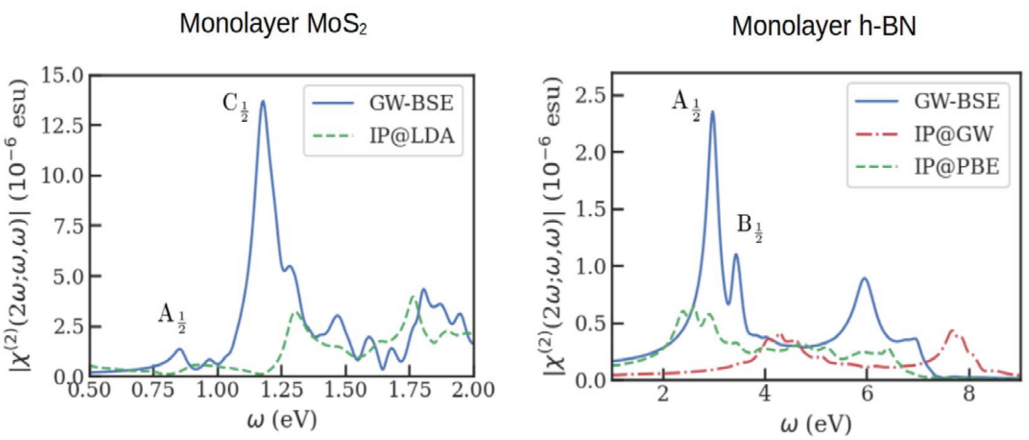


Figure 6: yyy component of the SHG susceptibility tensor for monolayer MoS_2 and monolayer h-BN. Results are computed at the level of GW-BSE, independent particle with LDA band energy, and independent particle with GW band energy levels.

In a recent work, we extended our real-time approach to study the high-harmonic generations, where the perturbative approach is not applicable [8]. We found that only when many-body effects are considered it is possible to reproduce the spectral features in the perpendicular response.

Exciton-phonon couplings in ultrafast exciton transitions in WS_2-MoS_2 heterobilayer

The role of exciton-phonon couplings in ultrafast intra-to-interlayer exciton transition in transition metal dichacolgenides (TMD) heterostructure remains under debate. Early studies based on time-dependent density functional approaches and non-adiabatic molecular dynamics suggests electron-hole and electron-phonon couplings conspire to achieve the ultrafast intra-to-interlayer exciton conversion process. In Ref. [9] we studied exciton transition pathways due to exciton-phonon couplings. Exciton-phonon scattering pathways in TMD heterostrucutre are strongly influenced by the spin-valley locking nature of their electronic structure as shown in Fig. 3(a). A cartoon picture of the scattering process, where excitons exchange momentum via phonons are shown in Fig. 3(c). We employ an *ab initio* many-body perturbation theory approach, which explicitly accounts for the excitons and phonons in the heterostructure. Our large-scale first-principles calculations directly probe the role of exciton–phonon coupling in the charge dynamics of the WS2/MoS2 heterobilayer. We find that the exciton–phonon interaction induced relaxation time of photoexcited excitons at the *K* valley of MoS2 and WS2 is 67 and 15 fs at 300 K, respectively, as shown in Fig. 3 (b) and (d), which sets a lower bound to the intralayer-to-interlayer exciton transfer time and is consistent with experiment reports.

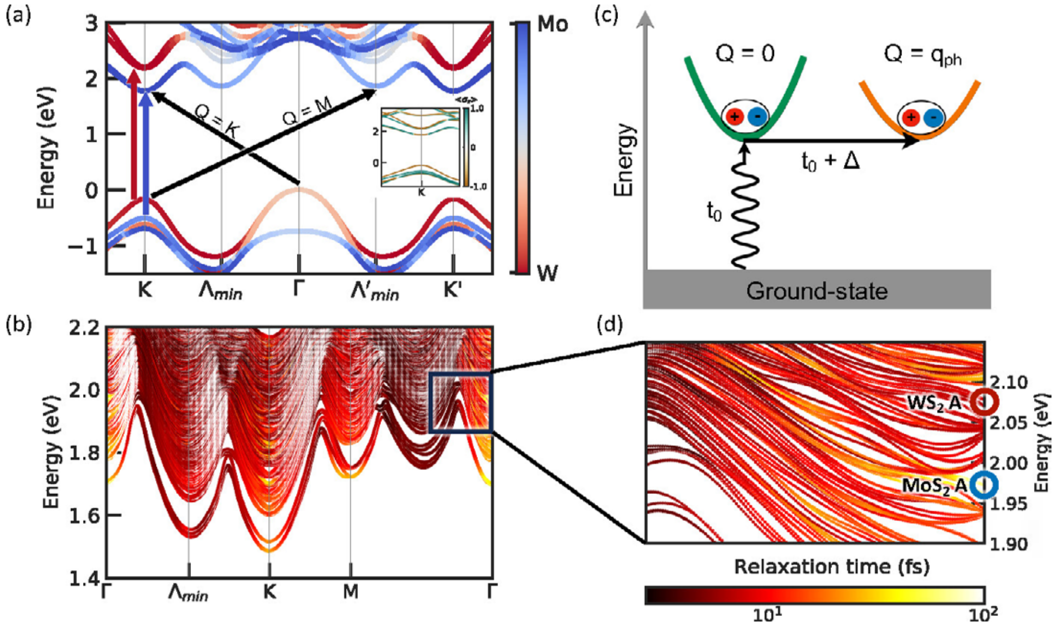


*Figure 7 (a) Electron band dispersion of the WS2/MoS2 heterostructure. Interband transitions corresponding to excitons with center of mass momentum **Q** = K and **Q** = M are shown with the labeled arrows. The inset shows a color map of the z-component of the spin expectation values of states near the K valley. (b) Exciton dispersion of both bound and resonant states of the WS2/MoS2 heterobilayer along a path of exciton center of mass momentum. Color indicates the value of the relaxation time due to exciton–phonon coupling at 300 K. (d) A zoom-in of panel (b) around the MoS2 and WS2 A excitons, which are indicated by blue and red circles, respectively. (c) Schematic representation of phonon-mediated exciton scattering process.*

Our analysis indicates that electron-hole correlations induce nonlocal distribution of electron or hole amplitude in reciprocal space and facilitate novel transfer pathways that are otherwise inaccessible to noninteracting electrons and holes. It would be interesting to simulate exciton Boltzmann dynamics with exciton-phonon scatterings. By directly comparing numerical simulation results with the time-resolved angle-resolved photoemission experiments we hope to further advance our understanding in exciton dynamics and provide essential knowledge for designing novel optoelectronic devices.

[1] M. Rohlfing, S. G. Louie, Electron-hole excitations and optical spectra from first principles. *Phys. Rev. B Condens. Matter Mater. Phys.* **62**, 4927–4944 (2000)
[2] Y. R. Shen, The Principles of Nonlinear Optics. Wiley-Interscience (2002).
[3] Robert W. Boyd, Nolinear Optics. Academic Press (2020)
[4] Yu-Tzu Chang and Yang-Hao Chan, Diagrammatic approach to excitonic effects on nonlinear optical response. Phys. Rev. B

109, 155437 (2024)
[5] Y.-H. Chan, D. Y. Qiu, F. H. Jornada, S. G. Louie, Giant exciton-enhanced shift currents and direct current conduction with subbandgap photo excitations produced by many-electron interactions. *Proc. Natl. Acad. Sci. U.S.A. 118, e1906938118 (2021)*
[6] Yi-Shiuan Huang, Yang-Hao Chan, and Guang-Yu Guo, Large shift currents via in-gap and charge-neutral excitons in a monolayer and nanotubes of BN. Phys. Rev. B 108, 075413 (2023)
[7] Jiawei Ruan, Yang-Hao Chan, and Steven G. Louie, Excitonic effects in nonlinear optical responses: Exciton-state formalism and first-principles calculations, arXiv:2310.09674
[8] Victor Chang Lee, Lun Yue, Mette B. Gaarde, Yang-hao Chan, and Diana Y. Qiu, Many-body enhancement of high-harmonic generation in monolayer MoS_2. Nat. Commun. 15, 6228 (2024)
[9] Yang-hao Chan, Mit H. Naik, Jonah B. Haber, Jeffrey B. Neaton, Steven G. Louie, Diana Y. Qiu, and Felipe H. da Jornada, Exciton–Phonon Coupling Induces a New Pathway for Ultrafast Intralayer-to-Interlayer Exciton Transition and Interlayer Charge Transfer in WS_2–MoS_2 Heterostructure: A First-Principles Study.
Nano Lett. 2024, 24, 26, 7972–7978.

Quantum criticality and non-Fermi liquid in correlated electron systems

Professor

Chung-Hou Chung

Center Scientist:

National Yang Ming Chiao Tung University

Condensed Matter Theory

- The scaled-invariant Planckian metal and quantum criticality in $Ce_{1-x}Nd_xCoIn_5$, Yung-Yeh Chang, Hechang Lei, C. Petrovic, and Chung-Hou Chung Nature Commun. 14 (581) (2023)

The mysterious Planckian metal state, showing perfect T-linear resistivity associated with universal scattering rate, $1/\tau = \alpha\, k_B T/\hbar$ with $\alpha \sim 1$, has been observed in the normal state of various strongly correlated superconductors close to a quantum critical point. However, its microscopic origin and link to quantum criticality remains an outstanding open problem. Here, we observe quantum-critical T/B-scaling of the Planckian metal state in resistivity and heat capacity of heavy-electron superconductor $Ce_{1-x}Nd_xCoIn_5$ in magnetic fields near the edge of anti-ferromagnetism at the critical doping xc ~ 0.03. We present clear experimental evidences of Kondo hybridization being quantum critical at x_c. We provide a generic microscopic mechanism to qualitatively account for this quantum critical Planckian state within the quasi-two dimensional Kondo-Heisenberg lattice model near Kondo breakdown transition. We find α is a non-universal constant and depends inversely on the square of Kondo hybridization strength. Perfect T-linear resistivity associated with universal scattering rate: $1/\tau = \alpha k_B T/(h/2\pi)$ with $\alpha \sim 1$, so-called Planckian metal state, has been observed in the normal state of a variety of strongly correlated superconductors close to a quantum critical point. However, the microscopic origin of this intriguing phenomena and its link to quantum criticality still remains an outstanding open problem. In this work, we observe the quantum-critical T/B-scaling of the Planckian metal state in the resistivity and heat capacity of heavy-electron superconductor $Ce_{1-x}Nd_xCoIn_5$ in magnetic fields near the edge of anti-ferromagnetism, driven by critical Kondo hybridization at the critical doping $x_c \sim 0.03$. We further provide the first microscopic mechanism to account for the Planckian state in a quantum critical system based on the critical charge fluctuations near Kondo breakdown transition at xc within the quasi-two-dimensional Kondo-Heisenberg lattice model. This mechanism simultaneously captures the observed universal Planckian scattering rate as well as the quantum-critical scaling and power-law divergence in thermodynamic observables near criticality. Our mechanism is generic to Planckian metal states in a variety of quantum critical superconductors near Kondo destruction. **Significance:** (i). We provide the first microscopic mechanism to account for the Planckian state in a quantum critical system. (ii). This mechanism simultaneously captures the observed universal Planckian scattering rate as well as the quantum-critical scaling and power-law divergence in thermodynamic observables near criticality. Our mechanism is generic to Planckian metal states in a variety of quantum critical superconductors near Kondo destruction. (iii). Due to this work, I have been invited to attend the prestigious workshops in world's leading physics institutes: the Aspen Center for Physics (USA), and KITP, Santa Barbara (USA), and several invited talks in important international conferences. Taiwan's NSTC hosted a press conference in Aug. 16, 2023 to highlight this work.

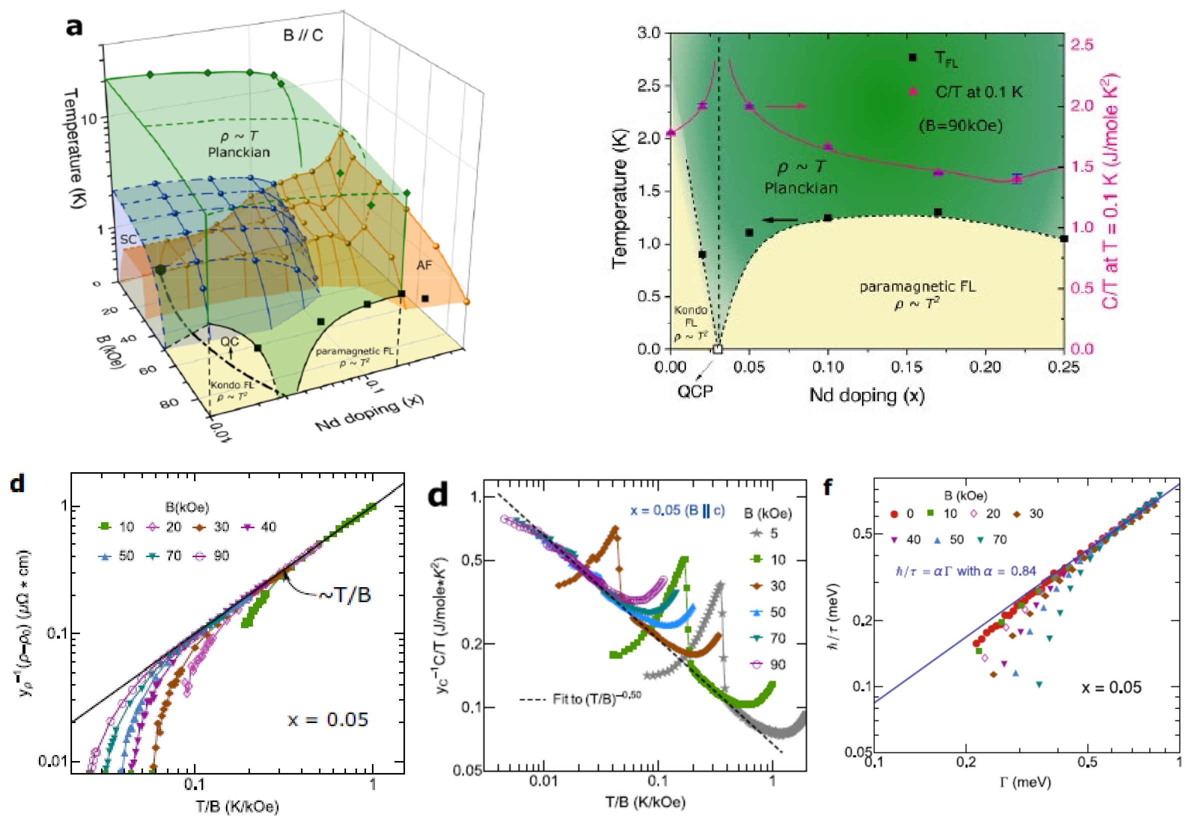


Figure 1. Top: Finite temperature phase diagrams of the rare-earth heavy-fermion superconductor Ce1-xNdxCoIn5 as functions of magnetic fields and Nd doping (Top Left) and as a function of Nd doping at a fixed magnetic field (Top Right). Bottom: The Planckian strange metal state showing quantum critical behaviors in electrical resistivity (Bottom Left), electron scattering rate (Bottom Middle), and specific heat coefficient (Bottom Right).

- Proximity induced charge density wave in a graphene/1T-TaS2 heterostructure, Michael A. Altvater, Seng-Hsiung Hung, Nikhil Tilak, Choong-Jae Won, Guohong Li, Sang-Wook Cheong, **Chung-Hou Chung***, Hrng-Tay Jeng*, Eva Y. Anderi*, Nature Communications 15, 8056 (2024).

The proximity-effect, whereby materials in contact appropriate each other's electronic-properties, is widely used to induce correlated states, such as superconductivity or magnetism, at heterostructure interfaces. Thus far however, demonstrating the existence of proximity-induced charge-density waves (PI-CDW) proved challenging. This is due to competing effects, such as screening or co-tunneling into the parent material, that obscured its presence. Here we report the observation of a PI-CDWin a graphene layer contacted by a 1T-TaS2 substrate. Using scanning tunneling microscopy (STM) and spectroscopy (STS) together with theoretical-modeling, we show that the coexistence of a CDW with a Mott–gap in 1T-TaS2 coupled with the Dirac-dispersion of electrons in graphene, makes it possible to unambiguously demonstrate the PI-CDW by ruling out alternative interpretations. Furthermore, we find that the PI-CDW is accompanied by a reduction of the Mott gap in 1T-TaS2 and show that the mechanism underlying the PI-CDW is well-described by short-range exchange-interactions that are distinctly different from previously observed proximity effects. **Significance:** (i). We unambiguously demonstrate the PI-CDW by ruling out alternative interpretations; (ii). We find that the PI-CDW is accompanied by a reduction of the Mott gap in 1T-TaS2 and show that the mechanism underlying the PI-CDW is well-described by short-range exchange-interactions that are distinctly different from previously observed proximity effects. I carried out the mean-field calculations.

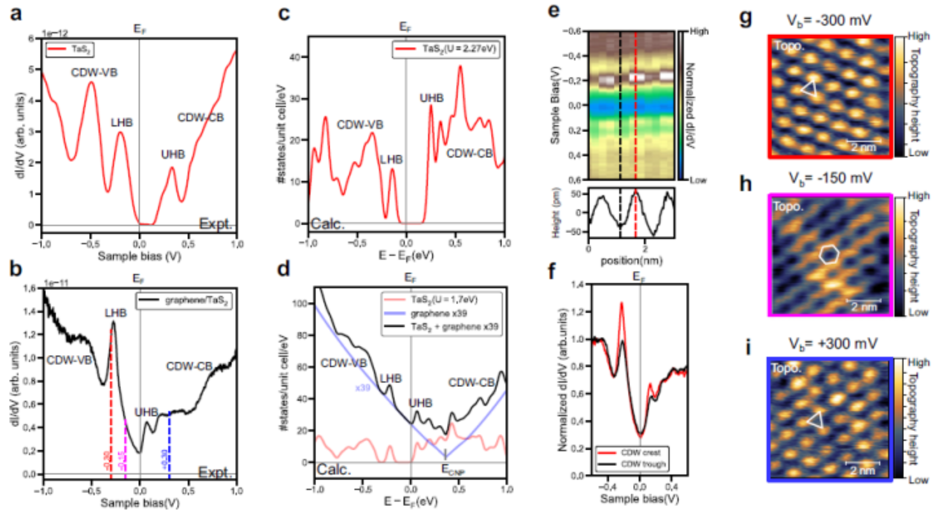


Figure 2. Left: STM of graphene covered 1T-TaS_2.

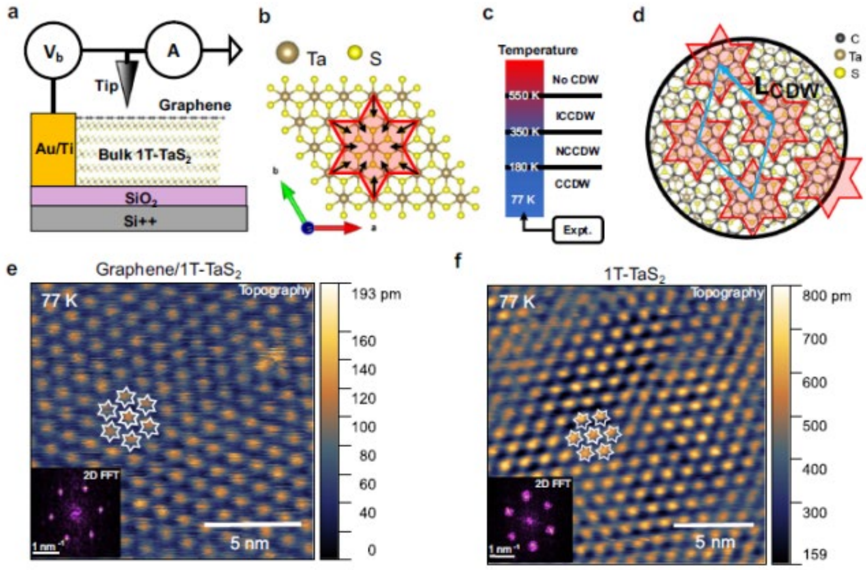


Figure 2. Right: Effects of interactions between graphene and 1T-TaS2.

- A mechanism for quantum-critical Planckian metal phase in high-temperature cuprate superconductors, Yung-Yeh Chang, Khoe Van Nguyen, Kim Remund, and Chung-Hou Chung∗, arXiv:2406.14858 (Reports on Progress in Physics, under review).

The mysterious metallic phase showing perfect T-linear resistivity and a universal scattering rate $1/\tau = \alpha_P\, k_B T/\hbar$ with an almost universal constant prefactor $\alpha_P \sim 1$ and logarithmic-in-temperature singular specific heat coefficient, so-called “Planckian metal phase” was observed in various high-Tc cuprate superconductors over a finite range in doping. Revealing the mystery of the Planckian metal state is believed to be the key to understanding the mechanism for high-Tc superconductivity. Here, we propose a generic microscopic mechanism for this state based on quantum-critical local bosonic charge Kondo fluctuations coupled to both spinon and a heavy conduction-electron Fermi surfaces within the heavy-fermion formulation of the slave-boson t-J model. By a controlled perturbative renormalization group analysis, we examine the competition between the pseudogap phase, characterized by Anderson’s Resonating-Valence-Bond spin-liquid, and the Fermi-liquid state, modeled by the electron hoping (effective charge Kondo effect). We find a quantum-critical metallic phase with a coupling-constant independent universal Planckian $\hbar\omega/k_B T$ scaling in scattering rate near an extended localized-delocalized (pseudogap-to-Fermi liquid) charge-Kondo breakdown transition. The d-wave superconducting ground state emerges near the transition. Unprecedented qualitative and quantitative agreements are reached between our theoretical predictions and various experiments, including optical conductivity, universal doping-independent field-to-temperature scaling in magnetoresistance, specific heat coefficient, marginal Fermi-liquid spectral function observed in ARPES, and Fermi surface reconstruction observed in Hall coefficients. Our mechanism offers a microscopic understanding of the quantum-critical Planckian metal phase observed in cuprates and its link to the pseudogap, d-wave superconducting, and Fermi liquid phases. It paves the way and offers a promising route for understanding how d-wave superconductivity emerges from such a strange metal phase in cuprates–one of the long-standing open problems in condensed matter physics since 1990s–as well as shows a broader implication for the Planckian strange metal states observed in other correlated unconventional superconductors.

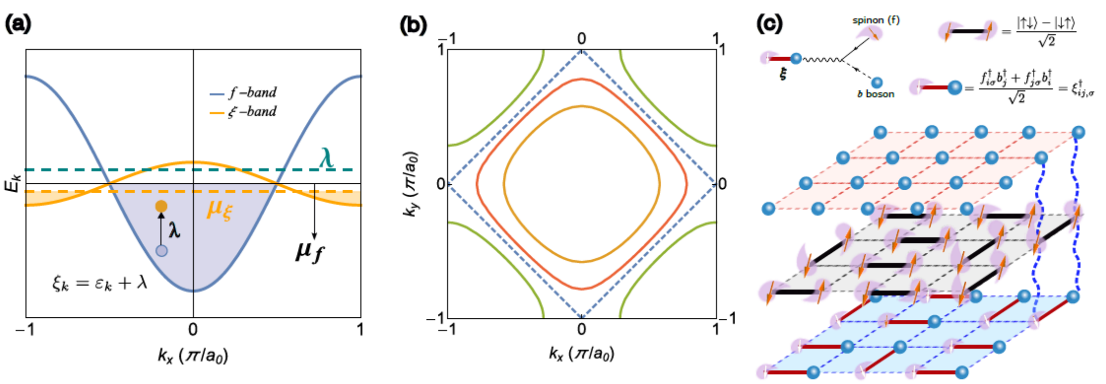


Figure 3. (a) Kondo hybridization between spinon and heavy-electron bands. (b) Fermi surfaces of spinon and heavy-electron bands. (c) Schematic plot of strange-metal state in terms of spinons, holons, and electrons.

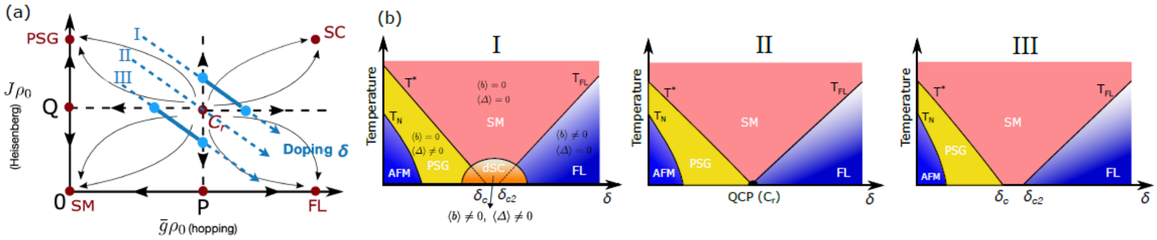


Figure 4. Renormalization Group (RG) flow and RG phase diagrams of our model.

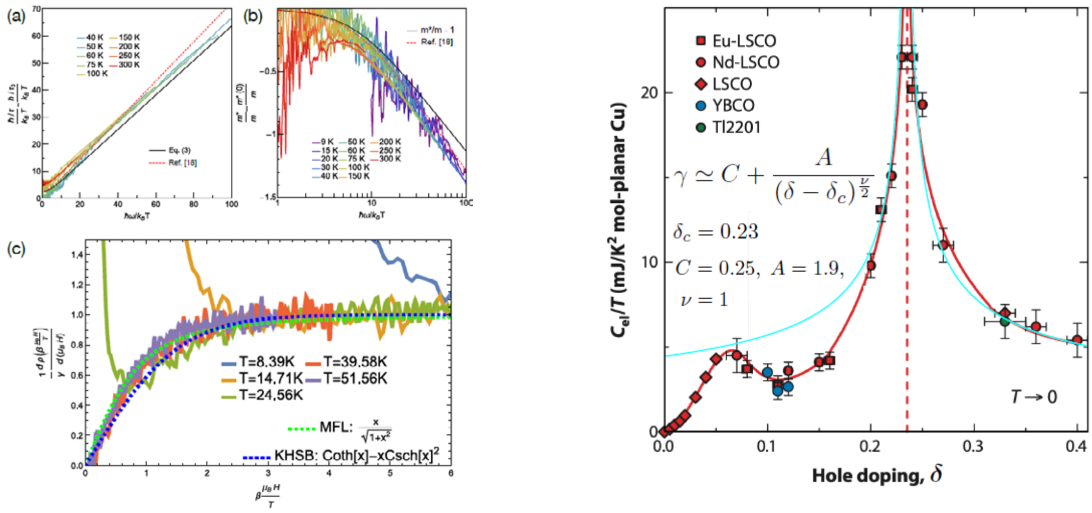
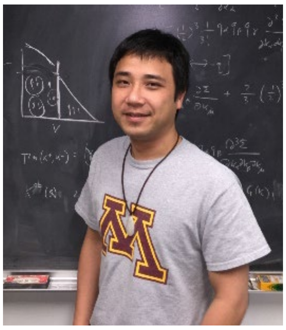


Figure 5. Left: Theoretical and experimental results on quantum critical scaling of the Planckian metal state in cuprates in scattering rate (a), electron effective mass (b), and magneto-resistivity. Right: Power-law divergence of specific heat coefficient at the pseudogap quantum critical point.

Exploration of Topological Phase Transitions in Honeycomb Ferromagnets Based on Self-Consistent Spin-Wave Theory



Associate Professor

Chien-Te Wu

Center Scientist

National Yang Ming Chiao Tung University

Condensed Matter Physics

We investigate topological phase transitions in two-dimensional (2D) honeycomb ferromagnets, which are materials with promising potential for spintronic applications. Spintronics focuses on using the "spin" of particles, a fundamental form of angular momentum, to carry information instead of relying on electronic charge. Honeycomb ferromagnets have unique properties that allow them to transport spin information with minimal energy loss since the spin-carrying particles, known as magnons, are charge-neutral and generate little to no heat during propagation. These characteristics make honeycomb ferromagnets ideal candidates for energy-efficient technology [1].

Our research explores phase transitions in honeycomb ferromagnets, with a specific focus on "topological" phase transitions. Phase transitions typically involve a change in the state of a material, like water turning into ice. In our study, a topological phase transition represents a change in the spin-carrying properties of the material, which are influenced by the material's structure and internal interactions. These transitions are particularly interesting because they can lead to the creation of robust, protected spin states that are highly resistant to external disturbances, making them ideal for use in stable spintronic devices [2].

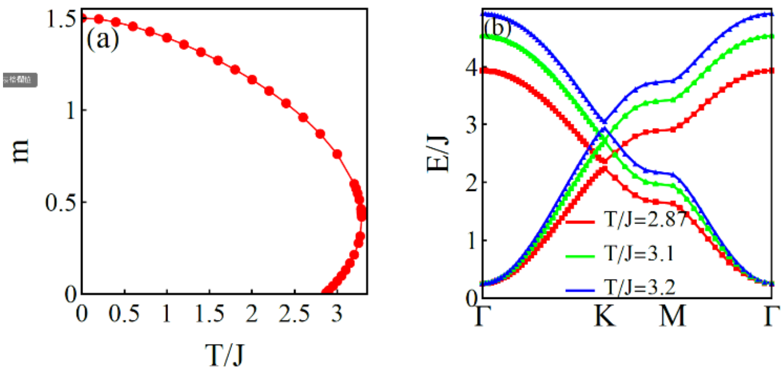


Fig. 8: (a) Magnetization as a function of temperature, exhibiting a first-order phase transition with an unphysical bend-back feature. (b) The corresponding magnon bands for the lower branch of the magnetization curve at three different temperatures.

To investigate these transitions, we used a theoretical approach called self-consistent renormalized spin-wave theory (SRSWT). Unlike traditional models that might neglect magnon-magnon interactions, SRSWT allows us to take these interactions into account, which gives a more realistic and accurate view of the system's behavior. By incorporating magnon interactions, we can predict the topological transition temperature, denoted as T_C, and explore how it relates to the Curie temperature T_{Curie}, the temperature at which a material loses its magnetic ordering.

One of the main results of our study is the determination of T_C, which is distinct from the Curie temperature. This distinction is crucial because it allows us to predict conditions under which these topological phase transitions can be experimentally observed, where T_C is lower than T_{Curie}. Furthermore, we found that an effect known as the Dzyaloshinskii-Moriya interaction (DMI) plays a critical role in these materials. The DMI acts similarly to spin-orbit coupling in electronic systems, introducing an energy gap at the Dirac points in the magnon band structure. This energy gap is essential for stabilizing topologically protected edge states—localized magnon modes that can contribute to a phenomenon called the thermal Hall effect. This effect is observable as a transverse heat flow that could potentially be used for thermal management in spintronic devices.

Another important aspect of our work is addressing the nature of the magnetic phase transition in honeycomb ferromagnets. This transition is of a second-order nature, meaning it occurs smoothly without a discontinuous jump in magnetization. However, we found that the SRSWT model, while providing a detailed view of magnon interactions and topological properties, inaccurately predicts a first-order transition in certain scenarios. This discrepancy arises due to inherent limitations in the SRSWT framework, which does not fully account for the kinematic constraints in the system. Despite this limitation, SRSWT remains valuable for approximating the conditions under which topological phase transitions can be observed, but our findings highlight the need for future models to refine these predictions. Accurately modeling these second-order transitions is essential, as they offer enhanced stability for applications, especially in environments with varying temperature and magnetic conditions.

This study contributes to the broader field of spintronics by providing insights into how topological magnonic states can be stabilized and manipulated in 2D honeycomb ferromagnets. These findings lay the groundwork for future experimental studies and practical applications, especially in the design of devices that use magnons to carry spin information in a highly stable and energy-efficient way. Further research could explore the effects of similar interactions in other lattice structures, such as kagome or triangular lattices, and assess experimental realizations in materials like CrI_3 [4], which exhibit similar magnetic properties. Overall, our results bring us closer to the development of efficient, robust spintronic devices that leverage topological protection for reliable data storage and transfer in next-generation technologies.

[1] F. Zhuo, J. Kang, A. Manchon, and Z. Cheng, Advanced Physics Research, 2300054.
[2] Y.-S. Lu, J.-L. Li, and C.-T. Wu, Phys. Rev. Lett. 127, 217202 (2021).
[3] L. Chen, J.-H. Chung, M. B. Stone, A. I. Kolesnikov, B. Winn, V. O. Garlea, D. L. Abernathy, B. Gao, M. Augustin, E. J. G. Santos, and P. Dai, Phys. Rev. X 11, 031047 (2021).

Finite-Size Scaling of 2D Classical System via Tensor Network

Professor

Pochung Chen

Center Scientist

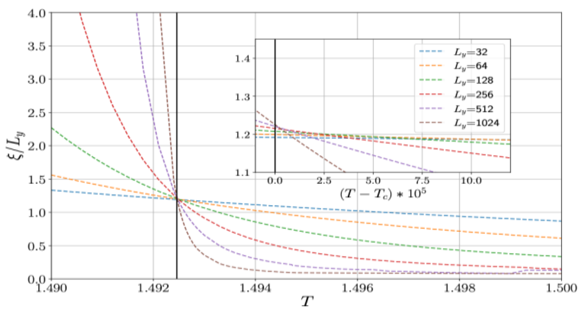
National Tsing Hua University

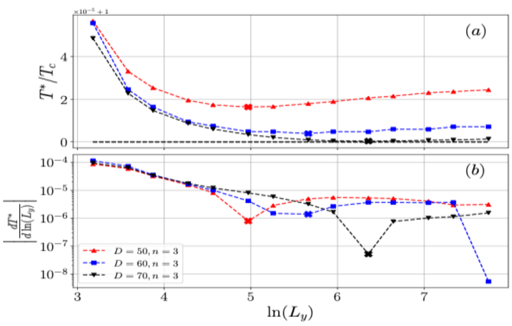
Computational Physics

In this series of works, we aim to explore deep connection between tensor network renormalization method and real-space renormalization group method. We apply conventional finite-size scaling analysis and use tensor network method to evaluate physical quantities. We consider an infinite strip of finite width and use tensor network method to evaluate approximately the transfer matrix and then the physical quantities. Here the bond-dimension D becomes a control parameter in additional to the system size L. It is commonly believed that a finite bond-dimension induced an effective length scale which scales as D^k. This becomes a two length-scales scaling problem. For a fixed D, when L is small, we expect that the system is described by the conventional finite-size scaling theory. On the other hand, when L is larger the system will crossover to the finite-entanglement scaling regime. Based on the real-space renormalization group concept, we propose that for any quantity Q, one should monitor *dlnQ/dlnL* and use the system size at which it reaches its first local minima as the best system size to estimate Q.

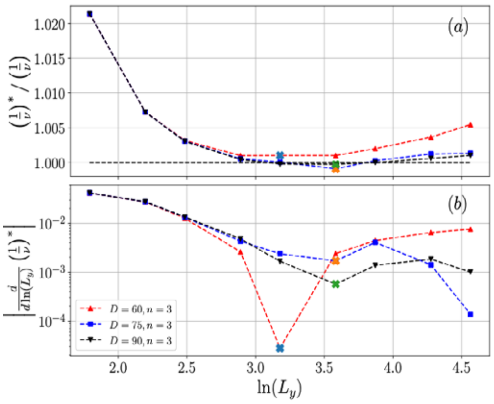
We have applied this idea to study 2D classical Ising model and 3-state clock model. We first investigate the dimensionless quantity ξ/L where ξ is the correlation length. As shown in Fig.1, we find that it crosses near T_c but the crossing point will draft. We hence use the finite-size scaling of the crossing point of to determine the critical temperature Tc as shown in Fig.2.

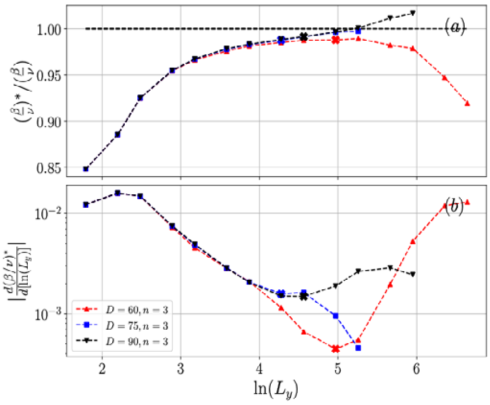
We fine that the critical temperature can be determined with extremely high accuracy, the error is at the order of 10^{-7}. To estimate the critical exponents $\frac{1}{\nu}, \frac{\beta}{\nu}, \frac{\alpha}{\nu}$, we use the slope of the ξ/L, the magnetization m, and the specific heat c_v respectively. As an example, the Fig.2 we show the results for the 3-state Potts model. For Ising model extremely high accuracy is obtained, with error at the order of 10^{-5}, 10^{-4}. For 3-state Potts model, the relative error is at the order of 10^{-4}, 10^{-3}. The accuracy is not as high as Ising model, but still very accurate. This is expected since 3-state Potts model is a



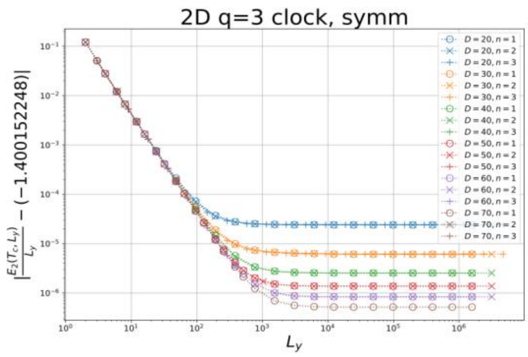


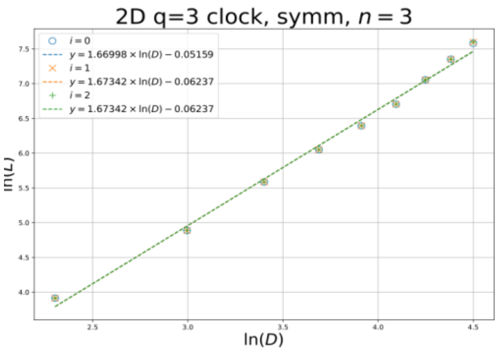
more complex model with higher central charge in the corresponding conformal field theory.





Finally, we study how the crossover length scales with the bond dimension. We first numerically estimate the free energy density in the thermodynamic limit. For a fixed *D*, we find that the free energy density will saturate at an effective D-dependent length *L(D)*, as shown in Fig.3(left). Then from a log-log plot as shown in Fig.3(right) we find $L(D) \propto D^{\kappa}$ and the value of fitted *k* is consistent with the expectation from conformal field theory.





1. Ching-Yu Huang, Sing-Hong Chan, Ying-Jer Kao, **Pochung Chen**, *Tensor Network Based Finite-Size Scaling for Two-Dimensional Classical Models*, Phys. Rev. B 107, 205123 (2023).

2. Debasmita Maiti, Sing-Hong Chan, **Pochung Chen**, *Tensor Network Finite-Size Scaling for Two-Dimensional 3-state Clock Model* arXiv:2312.14002.

Coexistence of superconductivity with partially filled stripes in the Hubbard model

Assistant Professor

Chia-Min Chung

Center Scientist

National Sun Yat-sen University

Condensed Matter Physics

1. Introduction

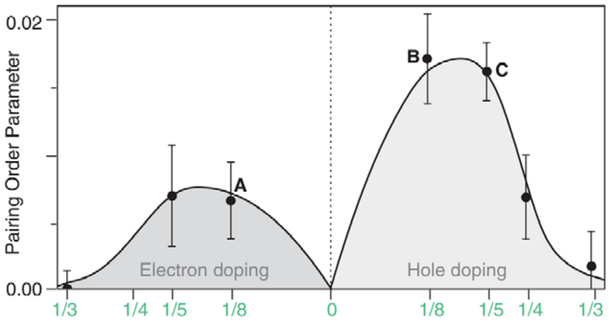
Whether the two-dimensional Hubbard model qualitatively captures the essential physics of the high-temperature superconducting cuprates has been long debated since shortly after these materials were discovered. Answering this question has proved to be especially difficult because the ground states of the models have been shown to be exceptionally sensitive to small changes in the model terms and parameters, with competing or cooperating charge, spin, and superconducting (SC) orders. The relevant model parameters are in the most difficult regime – moderately strongly-coupled – where most approaches struggle. The frequent presence of stripes in the ground states increases the sizes of the clusters needed to extrapolate to the thermodynamic limit. In our work (see Ref. [1]), we study the ground states of the two-dimensional Hubbard model with next-nearest neighbor hopping. In connection to the typical phase diagram of cuprates, the next-nearest neighbor hopping is necessary to account for the particle-hole asymmetry and the band structures.

2. Rationale

We employ two powerful modern computational methods – the density matrix renormalization group (DMRG) and the constrained path (CP) auxiliary field quantum Monte Carlo (AFQMC) methods – which are particularly complementary to each other. DMRG provides the most accurate and reliable results when applied on narrow cylinders. CP-AFQMC can be applied to both wider cylinders and toruses, and the underlying approximation of CP is unrelated to the low entanglement approximation of DMRG. Their quantitative handshake proved to be crucial for uncovering the delicate nature of the stripe correlations. Despite the extreme sensitivity of the system, we find that the physical quantities computed from these methods are quantitatively consistent for narrow cylinders, validating the use of CP-AFQMC for wider systems. The wider cylinders studied with CP-AFQMC allow extrapolation to the thermodynamic limit, which is crucial for understanding the competition between pairing and stripes. We apply twist-averaged boundary conditions to reduce the finite-size effect as it provides an effective means to sample the low-lying states and reduce the impact of rare events of accidental degeneracy.

3. Results

We find superconductivity in both the electron- and hole-doped regimes, and in both regimes, we find dome-like d-wave pairing order which resembles the Tc domes in the typical phase diagram of cuprates, as shown in Fig.1. We expect this zero-temperature property to be loosely connected to the transition temperature Tc most readily observed experimentally. The pairing order parameter is significantly larger in the hole-doped region than in the electron-doped region, which is also consistent with the phase diagram of cuprates. On the hole-doped side, we find the coexistence of superconductivity with fractionally filled stripe correlations, with nominal stripe fillings in the range 0.6-0.8 in sufficiently large sizes. On the electron-doped side, at lower dopings, uniform or weakly modulated antiferromagnetism, along with uniform or weakly modulated doping, coexists with somewhat weaker superconductivity. These behaviors of spin and charge are again consistent with the phase diagram of the cuprates, where uniform AF correlations persist with substantial doping on the electron-doped side, but short or long-ranged incommensurate magnetism and stripes are observed starting at small doping on the hole-doped side. The corresponding states are shown in Fig.1A-C.



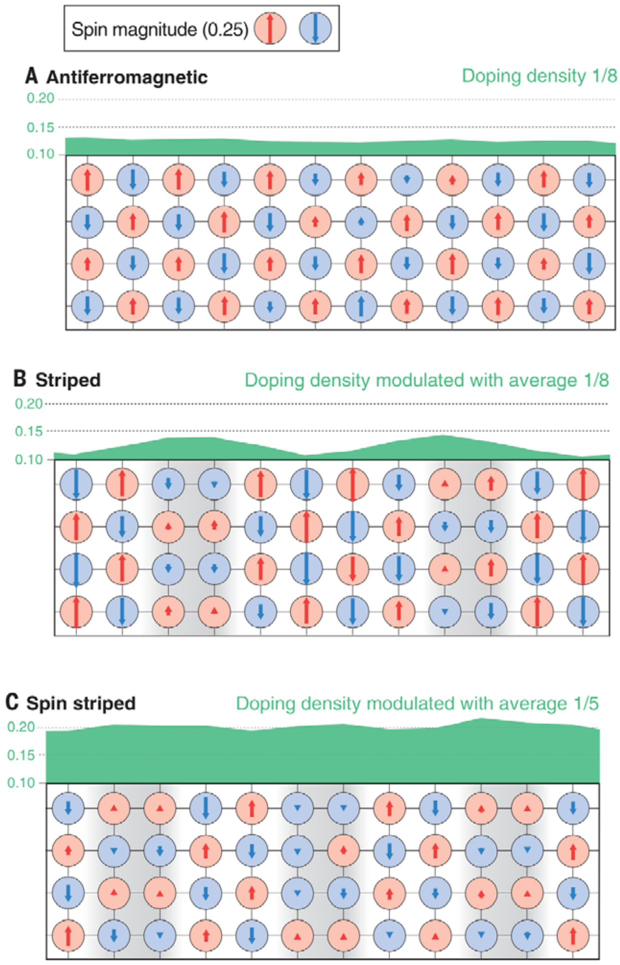


Fig. 1. The d-wave pairing-order parameter as a function of doping. Shown is the ground state for the hole-doped (t'=-0.2) and electron-doped (t'=+0.2) regimes. Representative spin and charge correlations are also shown for three parameter sets: A, B, and C.

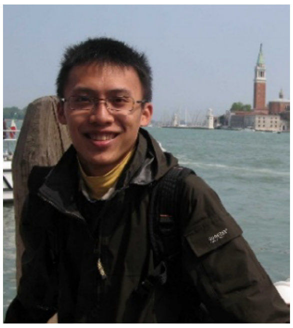
Another indication of the presence of long-range pairing order is illustrated by the number of electrons per stripe. In the models or parameter regimes on the hole-doped side where superconductivity is not present, one typically still finds strong indications of even numbers of holes in each stripe. In the superconducting region, as the size grows (wider cylinders), the integer-pair stripe states are no longer favored, and both systems tend to fractional stripe fillings. The general appearance of stripe orders on the larger systems with non-integral numbers of pairs indicates that pairs fluctuate between stripes, promoting long-distance phase coherence and thus superconductivity.

4. Conclusion

Can the single-band Hubbard model capture the qualitative physics, particularly the superconductivity, of the cuprates? Our calculations suggest that the answer is yes, that the Hubbard model with a next nearest-neighbor hopping t′ distinguishing between electron- and hole-doping captures the essential features of the charge, magnetic, and pairing orders. Other terms and effects not present in the Hubbard model may still play important quantitative roles. Nevertheless, it appears that qualitatively, the t-t′-U Hubbard model may have “the right stuff”.

[1] Coexistence of superconductivity with partially filled stripes in the Hubbard model
H Xu† , Chia-Min Chung† , M Qin, U Schollwöck, SR White, S Zhang
Science 384, eadh7691 (2024)

Quantum dynamics, topology, localization, and graph theory



Assistant Professor

Yi-Ping Huang

Center Scientist
National Tsing Hua University
Condensed Matter Physics

Why correlated quantum dynamics?

The study of correlated dynamics is a rapidly evolving interdisciplinary field, bringing together experts in quantum information science, quantum computing, and condensed matter theory.

A central question in this field is how information is scrambled during unitary time evolution. Typically, this process leads to thermalization, where information from the initial many-body wave function is preserved under the system's global unitary evolution. However, local operations cannot faithfully retrieve this information since arbitrary subsystems exchange information with their complements. Therefore, the close quantum system acts like its own bath that drives the system to equilibrium[1].

Although the concept of thermalization is well-supported by current numerical studies and experiments, there is no general proof of thermalization for arbitrary many-body quantum systems. In developing quantum technologies, avoiding thermalization is essential to manage information effectively within quantum systems, which is critical for algorithm development. Therefore, a key question shifts from understanding how a system thermalizes to how thermalization can be avoided and whether novel dynamical patterns might emerge for diverse applications.

Studying the emergent dynamical patterns in quantum many-body systems is inherently challenging. This complexity arises not only because of the interdisciplinary nature of the field but also from the limited understanding of the behavior of excited states. Traditional many-body physics often focuses on low-energy or ground-state phenomena, while correlated quantum dynamics focuses on unitary evolution, which demands insights into the full spectrum of eigenstates. Identifying mechanisms that transcend conventional equilibrium physics is therefore a primary challenge in this field.

We are especially interested in quantum systems with gauge constraints and spin-orbit coupled systems. The former is closely related to effective description of non-trivial entanglement pattern in equilibrium. The latter is the simplest non-trivial setting to understand how internal degrees of freedom could influence its dynamics.

Dynamics of quantum systems with gauge constraints

We have studied the dynamics of quantum systems with gauge constraints for several years. Previously, our work integrated theoretical models and computational tools to examine complex dynamics within lattice gauge theories through the lens of dynamical quantum phase transitions[2]. Here, unitary evolution is associated with partition function zeros—a fundamental concept in defining phase transitions in statistical mechanics.

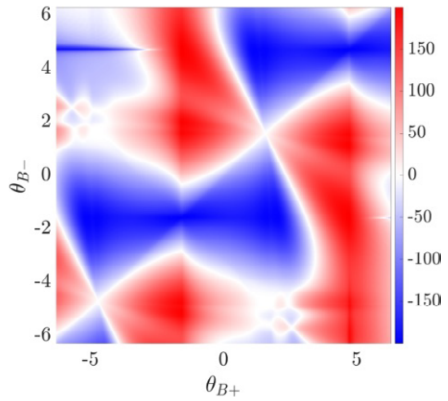
Recently, one branch of my research seeks to uncover universal mechanisms that prevent thermalization. Several classes of phenomena demonstrate deviations from thermalization, with our focus on two: many-body localization and many-body scars. We investigate these phenomena within lattice gauge theories, where gauge constraints produce unique dynamical effects.

Our research has also revealed disorder-free localization within a two-dimensional U(1) quantum link model[3]. Here, gauge sectors function as distinct disorder realizations, with the localization phenomenon associated with percolation transitions. Our work leverages quantum parallelism through a disorder-averaging process, where different gauge charge sectors interact in novel ways.

These constrained systems continue to yield surprising dynamical behavior. Recently, we identified a general mechanism for the formation of quantum many-body scars—unusual mid-spectrum eigenstates that evade thermalization[4]. We refer to these as interference-caged quantum many-body scars (ICQMBS), stemming from the generalization of topological localization in flat-band physics to the Fock space graph. Identifying ICQMBS has led us to explore graph automorphisms as a tool for understanding the stability of quantum many-body scars, opening new avenues in correlated dynamics[5].

Quantum dynamics and game theory

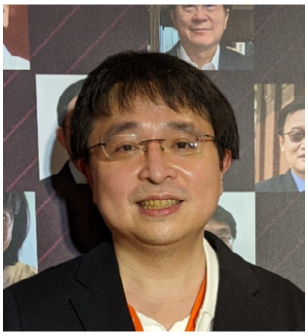
A second branch of my recent research examines interdisciplinary applications of quantum dynamics. One example involves Parrondo's paradox in classical game theory, where combining losing strategies produces a winning outcome. Using a quantum walk system, we created the simplest non-trivial setting to realize Parrondo's paradox through quantum interference[6] which can be realized in near term experiments. Below is the phase diagram for the Parrondo's paradox using the quantum coin's phase parameters θ_{B_-} and θ_{B_+} . The red region is the region where Parrondo's paradox is achieved.



1. D'Alessio, L., Kafri, Y., Polkovnikov, A. & Rigol, M. From quantum chaos and eigenstate thermalization to statistical mechanics and thermodynamics. Adv. Phys. **65**, 239–362 (2016).
2. Huang, Y.-P., Banerjee, D. & Heyl, M. Dynamical Quantum Phase Transitions in U(1) Quantum Link Models. Phys. Rev. Lett. **122**, 250401 (2019).
3. Karpov, P., Verdel, R., Huang, Y.-P., Schmitt, M. & Heyl, M. Disorder-Free Localization in an Interacting 2D Lattice Gauge Theory. Phys. Rev. Lett. **126**, 130401 (2021).
4. Chandran, A., Iadecola, T., Khemani, V. & Moessner, R. Quantum Many-Body Scars: A Quasiparticle Perspective. Annu. Rev. Condens. Matter Phys. **14**, 443–469 (2023).
5. Tan, T.-L. & Huang, Y.-P. Interference-caged quantum many-body scars: a

consequence of the Fock space topological localization. In preparation
6. Mittal, V. & Huang, Y.-P. Parrondo's paradox in quantum walks with inhomogeneous coins. Preprint at https://doi.org/10.48550/ARXIV.2407.16558 (2024).

Anomalous Giant Superradiance in Molecular Aggregates Coupled to Polaritons



Associate Research Fellow and Joint Associate Professor

Liang-Yan Hsu

Center Scientist
Academia Sinica
Theoretical Chemical Physics

In the realm of quantum electrodynamics and quantum optics, the concept of superradiance—first introduced by Dicke in 1954—has captivated researchers by describing how spaced molecules can emit light coherently, leading to enhanced emission rates. This fascinating phenomenon has been widely studied across various systems, including atoms, quantum dots, Bose-Einstein condensates, and especially molecular aggregates. Notably, Kasha et al. conducted a series of pioneering studies on excitons in molecular aggregates, focusing on Coulombic dipole-dipole interactions between monomers. Their works successfully explained experimental luminescence spectra during the 1950s and 1960s. A further significant advancement occurred in 1989 when Spano and Mukamel utilized a comprehensive quantum electrodynamics (QED) framework to investigate molecular aggregates, deriving the collective emission rate of the superradiant state and the corresponding energy levels in free space. In our recent study, my student Yi-Ting Chuang and I delve into a new type of this phenomenon: anomalous giant superradiance in molecular aggregates coupled to surface plasmon polaritons (SPPs) [1]. This investigation not only enriches the understanding of superradiance but also highlights the critical roles of counter-rotating interactions [2] and resonant dipole-dipole interactions [3].

Using macroscopic quantum electrodynamics (MQED) as our framework, we explore how polaritons can significantly amplify superradiance, deviating from the traditional Dicke N scaling law. Our analytical derivation reveals a general formula for the superradiance rate applicable across arbitrary dispersive and absorbing media, demonstrating that this phenomenon can yield rates an order of magnitude larger than conventional superradiance—even with small aggregates, such as those containing just ten monomers, as shown in Fig. 1.

A crucial aspect of our findings emphasizes the importance of intermolecular distances and transition dipole moments in modulating the spectral enhancement that drives giant superradiance. The interplay between dipole enhancement, grounded in previous famous theories, and spectral enhancement—a novel contribution from SPPs—forms the basis of our observed anomalies [1].

Moreover, we highlight the often-overlooked counter-rotating interactions within the quantum dynamics of multiple molecules. Traditionally, the rotating-wave approximation has been employed to simplify light-matter interactions; however, our analysis underscores that neglecting counter-rotating terms can lead to substantial deviations in intermolecular dipole-dipole interactions, particularly in the weak coupling regime. For instance, we analytical derived that these interactions converge to merely half of the expected Coulombic interactions in the non-retarded limit [2].

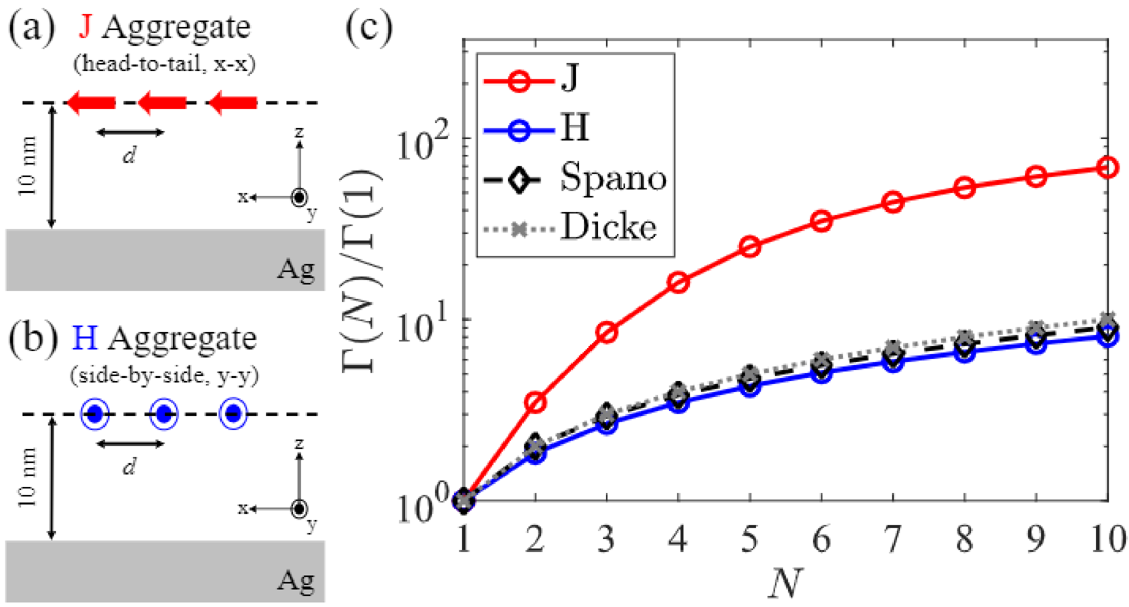


Fig. 1. Scheme of (a) J aggregate and (b) H aggregate above a silver surface. (c) N dependence of superradiance rate enhancement calculated from different theories. The red circle line shows that J aggregate can yield rates an order of magnitude larger than conventional superradiance derived from Spano's theory and Dicke's theory. Copyright 2019, American Physics Society [1].

This study opens new avenues for manipulating superradiance in molecular aggregates and invites further exploration of the fundamental mechanisms behind these phenomena, potentially impacting fields such as quantum optics and materials science. By integrating insights from both superradiance theory and counter-rotating interactions, we pave the way for future investigations into the intricate behaviors of light-matter interactions in complex dielectric environments.

[1] Y.-T. Chuang and L.-Y. Hsu, Anomalous giant superradiance in molecular aggregates coupled to polaritons, Phys. Rev. Lett. 133, 128001 (2024).

[2] Y.-T. Chuang and L.-Y. Hsu, Quantum dynamics of molecular ensembles coupled with quantum light: Counter-rotating interactions as an essential component, Phys. Rev. A 109, 013717 (2024).

[3] Y.-T. Chuang and L.-Y. Hsu, Microscopic theory of exciton–polariton model involving multiple molecules: Macroscopic quantum electrodynamics formulation and essence of direct intermolecular interactions, J. Chem. Phys. 160, 114105 (2024).

From Static to Dynamic: Advancing Our Understanding of Charge Transfer Processes in Complex Molecular Environments

Research Fellow

Chao-Ping (Cherri) Hsu

Center Scientist

Academia Sinica

Charge transfer

Charge transfer (CT) is a fundamental process in chemistry and biochemistry, playing a crucial role in various phenomena, including redox reactions, photosynthesis, and the operation of organic electronic devices. The rate of CT is largely governed by the electronic coupling between the donor and acceptor molecules and the reorganization energy associated with the transfer process. Understanding these factors is essential for developing efficient and high-performance materials for applications in organic electronics, energy storage, and catalysis.

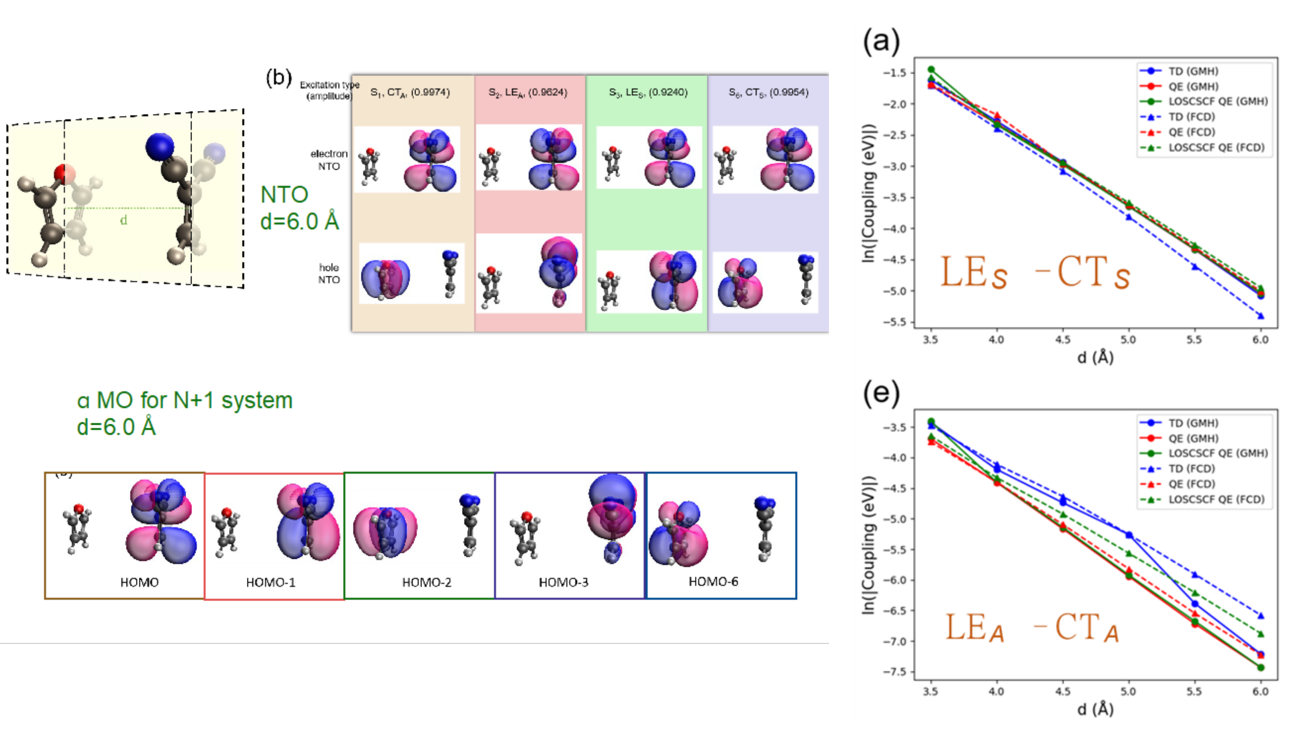


Figure 1. For a pair of donor-acceptor, the natural transition orbitals corresponds well to the molecular orbitals of N+1 system, with much better exponential-decay distance dependence.[1]

Traditionally, CT processes have been studied using theoretical frameworks such as Marcus theory and its extensions. These theories provide valuable insights into the relationship between the rate of CT and factors like driving force, reorganization energy, and electronic coupling. However, accurately calculating these parameters for complex systems can be computationally demanding, often requiring sophisticated quantum chemical methods. This has led to the exploration of alternative approaches, including machine learning (ML) and quasiparticle energy (QE) methods, to enhance the efficiency and accuracy of predicting CT properties, an area where Center Scientist Chao-Ping (Cherri) Hsu and her coworkers focused on. As a result, a comprehensive overview of Marcus theory and its applications to two-state photophysical processes, published as an invited book chapter (Hsu and Yang (2024))

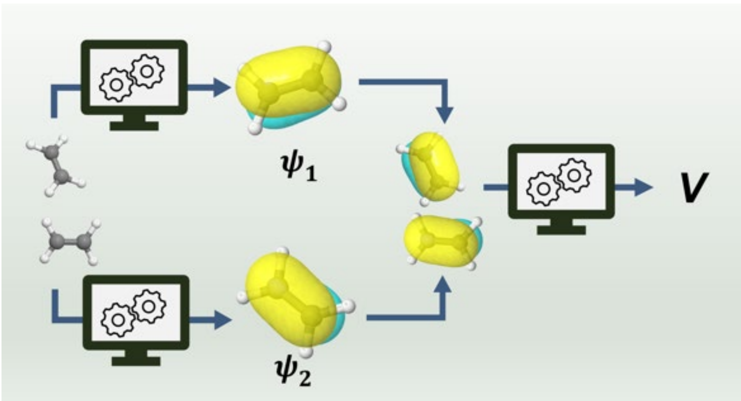


Figure 2. A schematic representation of our two-step ML model.[2]

The QE scheme is a computationally efficient approach for excited state energies, and it was extended to calculate ET couplings in excited states. Hsu and coworkers showed that their method accurately predicts couplings, particularly their exponential distance dependence, for a furan-DCNE complex. Their work presents a promising alternative to computationally expensive TDDFT methods for studying excited-state CT phenomena.[1]

Hsu and coworkers have also been addressing the challenge of efficiently predicting electronic coupling in molecular dimers crucial for understanding CT in organic semiconductors. The authors proposed a two-step ML scheme that accurately reproduces the distance dependence of electronic coupling in both ethylene and naphthalene dimers. This ML approach offers a significant speedup compared to traditional quantum chemical calculations, making it suitable for studying larger systems and screening potential CT materials.[2]

Given a good and efficient ML model, Hsu and coworkers further provided valuable insights into the dynamic disorder of electronic coupling, a crucial factor affecting CT rates in real systems. Using MD simulations and ML models, we investigated the influence of intermolecular motions on electronic coupling in ethylene and naphthalene dimers, highlighting the dominant role of low-frequency modes Their findings underscore the need to consider dynamic effects when modeling CT processes in complex environments.[3]

With MD simluation, Hsu and coworkers further challenged the common assumption of neglecting outer-sphere reorganization energy (λ_{out}) in nonpolar CT systems. The authors demonstrated that λ_{out} can be significant, even in nonpolar environments, and showed that it influences both the magnitude and temperature dependence of the overall reorganization energy. Their findings have implications for accurately modeling CT rates in a wide range of systems, including organic semiconductors and biological systems.[4]

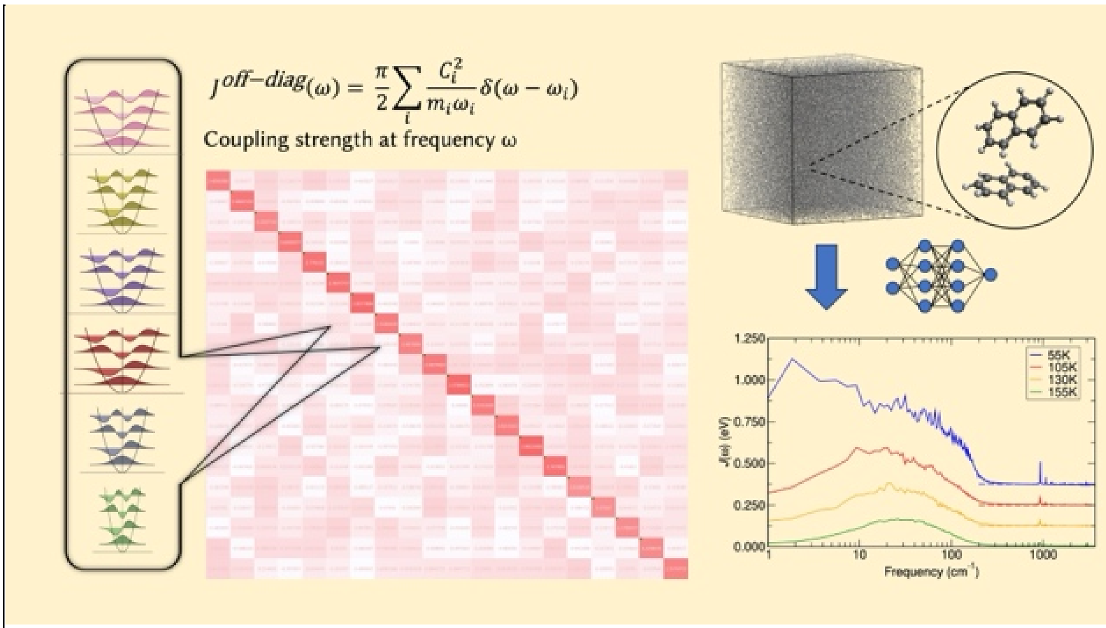


Figure 3. ML assisted off-diagonal dynamic disorder, with the off-diagonal spectral density function depicted as a projection to many Harmonic oscillators.[3]

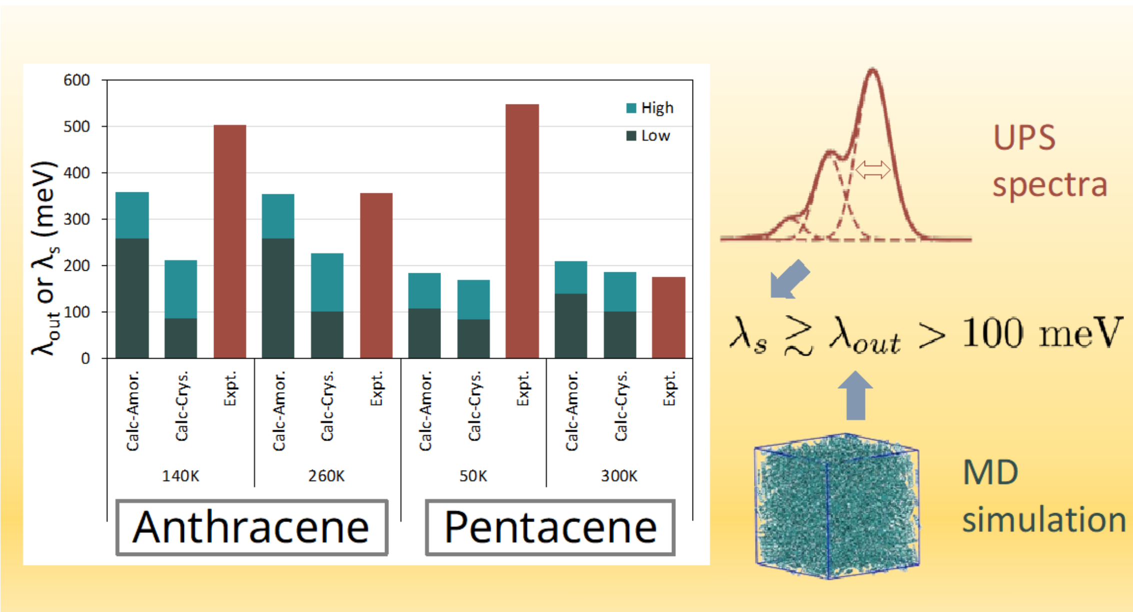


Figure 4. Estimated reorganization energies from experimental and simulational approaches.[4]

Meanwhile, the challenge of predicting the selectivity of chemical reactions with post-transition-state bifurcation (PTSB) energy surfaces, a phenomenon where the reaction pathway branches after the transition state, leading to multiple products, was also tackled by Hsu and coworkers. They demonstrated that KRR-aided QCT-MD is a robust and accurate method for predicting dynamic selectivity in such reactions, and it can be used to resolve the discrepancy between numerical *ab initio* molecular dynamics (AIMD) and intuitive model predictions (Figure 5). This approach provides a powerful tool for studying complex reaction mechanisms and designing new synthetic strategies.[5]

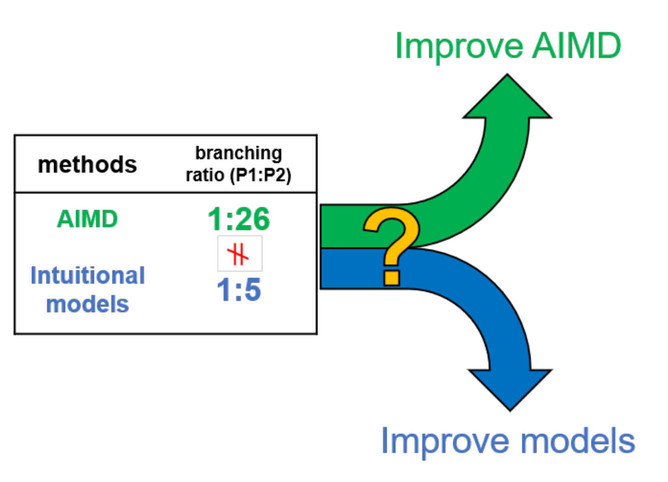


Figure 5. When there is a limited number of AIMD trajectories, the discrepancy between AIMD and intuitional model can arise from statistics. We have addressed the problem by offering ML enhanced AIMD statistics.[5]

In sum, Hsu and coworkers contribute significantly to the field of CT research. They introduce novel computational methodologies, such as KRR-aided QCT-MD, QE methods, and ML techniques, to address the challenges of predicting CT parameters accurately and efficiently. They also provide new insights into the dynamic nature of electronic coupling and the importance of considering λ_{out} even in nonpolar systems. These advancements enhance our understanding of CT processes and offer valuable tools for designing and developing new materials for various technological applications.

[1] K.-Y. Kuan, S.-H. Yeh, W. Yang, and C.-P. Hsu, "Excited-State Charge Transfer Coupling from Quasiparticle Energy Density Functional Theory," J. Phys. Chem. Lett. **15**(23), 6126–6136 (2024).

[2] H.-H. Lin, C.-I. Wang, C.-H. Yang, M.K. Secario, and C.-P. Hsu, "Two-Step Machine Learning Approach for Charge-Transfer Coupling with Structurally Diverse Data," J. Phys. Chem. A **128**(1), 271–280 (2024).

[3] Y.-S. Wang, C.-I. Wang, C.-H. Yang, and C.-P. Hsu, "Machine-learned dynamic disorder of electron transfer coupling," The Journal of Chemical Physics **159**(3), 034103 (2023).

[4] C.-H. Yang, C.-I. Wang, Y.-S. Wang, and C.-P. Hsu, "Non-negligible Outer-Shell Reorganization Energy for Charge Transfer in Nonpolar Systems," J. Chem. Theory Comput. **20**(16), 6981–6991 (2024).

[5] K.-Y. Kuan, and C.-P. Hsu, "Predicting Selectivity with a Bifurcating Surface: Inaccurate Model or Inaccurate Statistics of Dynamics?," J. Phys. Chem. A **128**(32), 6798–6805 (2024).

Avalanche Dynamics: A Deep Dive into Mesoscale Friction and Contact Line Motion

Professor

Pik-Yin Lai

Center Scientist
National Central University
Complex Systems

In the world of physics, where laws often appear universal, some natural phenomena defy simplification. One of these mysteries is the avalanche-like behavior observed in systems under stress, a phenomenon where minor perturbations can cause sudden, large-scale events. Our two recent studies—one exploring the nature of stick-slip friction at the mesoscale[1] and the other investigating the dynamics of a moving contact line[2]—have provided new insights into this behavior, revealing common statistical properties in seemingly unrelated systems. Let's delve into the fascinating interplay of friction and fluid dynamics, which brings forth a shared narrative of avalanche dynamics.

Nature's Dance of Stick-Slip: Friction at the Mesoscale:

Our combined theoretical and experimental studies[1], offers a fresh look at friction on a small scale. Typically, frictional movement between surfaces involves a series of tiny, localized "stick-slip" events, where surfaces momentarily lock together before slipping apart with a burst of energy. Using a novel atomic force microscopy (AFM) setup, we could observe these small-scale movements in unprecedented detail. By studying friction on a rough silicon carbide substrate, these intermittent "slips" are captured and key quantities are measured, such as the force at which slippage occurs (known as the depinning force) and the distance over which it happens.

A standout discovery in this work was that here indeed exists a critical regime in which stick-slip friction can be described by a common set of statistical laws of avalanche dynamics. For instance, the maximal force needed to trigger the local slips obeys the generalized extreme value distribution very well whereas the slip lengths are well-characterized by a power-law distribution, a hallmark of systems near a critical state, with the power-law exponent explained. Furthermore, the stick-slip motion of the scanning probe can be envisioned as a result of its center-of-mass moving in a random pinning force field described by an under-damped spring-block model subjected to a Brownian-correlated pinning force field. The model captures the essential physics of the stick-slip friction at mesoscale, providing a long-sought physical mechanism for the avalanche dynamics in stick-slip friction. In layperson's terms, the stick-slip statistical law means that smaller slips were more common, but occasionally, the system experienced a much larger slip that released significantly more energy. This observation supports a theoretical framework of avalanche dynamics, suggesting that frictional slippage doesn't occur in isolation but involves a cascading series of events influenced by neighboring points on the surface. Remarkably, this statistical behavior, captured at the mesoscale, reflects patterns seen in vastly different systems, from geological faults during earthquakes to soft materials under stress.

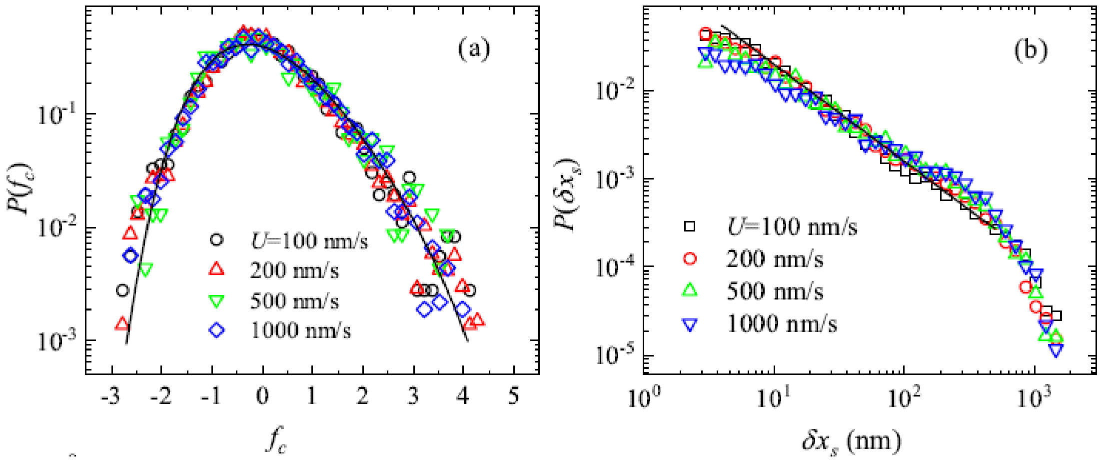


Fig. 1. Measured PDFs of the (a) normalized maximal force fc and (b) slip length δx_s for different scanning speeds U, using the quasi-1D probe. (Taken from [1]).

Avalanches at the Interface: The Contact Line Story

Our second study, by the same team, extends this concept to a different system: the movement of a contact line (CL) of a liquid interface. Imagine a tiny fiber dipped into a liquid. The point where the liquid meets the fiber—the contact line—doesn't move smoothly as the fiber is pulled but undergoes similar stick-slip events, influenced by the roughness and defects on the fiber surface. The experiments used a long-needle AFM probe to monitor the CL dynamics at an impressive level of detail, mapping out the tiny capillary forces that emerge as the CL momentarily sticks to defects on the fiber before slipping away.

Like the frictional stick-slip motion, it is found that the CL movement exhibited an avalanche-like pattern. The force needed to dislodge the CL from each defect followed a predictable statistical distribution, and the slip lengths mirrored the power-law distribution observed in the friction study. This shared behavior across different scales and contexts—solid-solid friction versus fluid-structure interaction—suggests that the mesoscale properties of surface roughness and pinning forces play a central role in shaping the avalanche dynamics. Our findings provide an accurate statistical description of the CL dynamics at mesoscale, which has important implications to a common class of problems involving stick-slip motion in a random defect or roughness landscape.

Both studies converge on the concept of avalanche dynamics, where individual pinning sites act as points of resistance, accumulating stress until they collectively "give way," triggering a cascade of slips. This shared behavior is fascinating because it reveals that the specifics of the material—whether solid or fluid—are less important than the underlying structure and interaction forces. In both cases, the dynamics can be understood within the framework of the Alessandro-Beatrice-Bertotti-Montorsi (ABBM) model, which describes systems with randomly distributed pinning sites and was initially applied to magnetic domain walls in soft magnets. By applying this model to both friction and CL systems, we offer a unified perspective on how such systems evolve under stress. Moreover, these findings highlight the role of randomness and heterogeneity in shaping natural processes. The roughness of the contact surfaces, whether in solid-solid friction or in liquid-solid interactions, introduces variations that the system cannot predict or control. Yet, when viewed as a whole, these individual variations combine to form predictable statistical patterns. These patterns provide insight into designing materials with tailored frictional properties or surfaces engineered to minimize fluid drag.

The implications of this research and possible applications are as broad as they are exciting. For instance, understanding mesoscale friction dynamics could improve technologies dependent on precise control over surface interactions, such as advanced robotics or nanoscale manufacturing. Similarly, insights into CL motion could influence a wide range of applications, from enhancing the efficiency of liquid transport in microfluidics to designing self-cleaning surfaces where controlled wetting properties are essential. More broadly, these studies remind us of the universality underlying complex systems. Whether we're looking at the way rocks shift during an earthquake or how a droplet slides down a window, the principles guiding these actions are deeply connected. Each slip, each release of tension, contributes to a dance that balances unpredictability with deeply rooted patterns—revealing that even in chaos, nature is guided by rules.

.

[1] "Statistical laws of stick-slip friction at mesoscale", C. Yan, H.Y. Chen, Pik-Yin Lai, P. Tong, Nature Comm. 14, 6221 (2023). (See also: https://physicscommunity.nature.com/posts/statistical-laws-of-stick-slip-friction-at-mesoscale?channel_id=behind-the-paper)
[2] "Avalanches and extreme value statistics of a moving contact line", C. Yan, D. Guan, Y. Wang, H.Y. Chen, Pik-Yin Lai, P Tong, Phys. Rev. Lett. 132, 084003-1~6 (2024). (Editor's Suggestion)

Statistical model and universality class of transitional turbulence

Assistant Research Fellow

Hon-Yan Shih

Center Scientist

Institute of Physics, Academia Sinica

Complex Systems

Turbulence is a common phenomenon in nature and has significant industrial relevance. When turbulence starts to develop, flow dynamics become highly nonlinear and complex, a process that remains not fully understood since Reynolds' original observations over 140 years ago. The state of fluid flow is characterized by the Reynolds number ($Re = UD/\nu$), where U is velocity, D is length, and ν is viscosity. In pipe flow, when Re exceeds approximately 2000, the flow transitions from laminar to localized turbulent regions, or "puffs," which gradually decay. As Re increases, these puffs become more persistent and begin to split, exhibiting spatiotemporal intermittency. The transitional point is defined by the balance between puff decay and splitting [1].

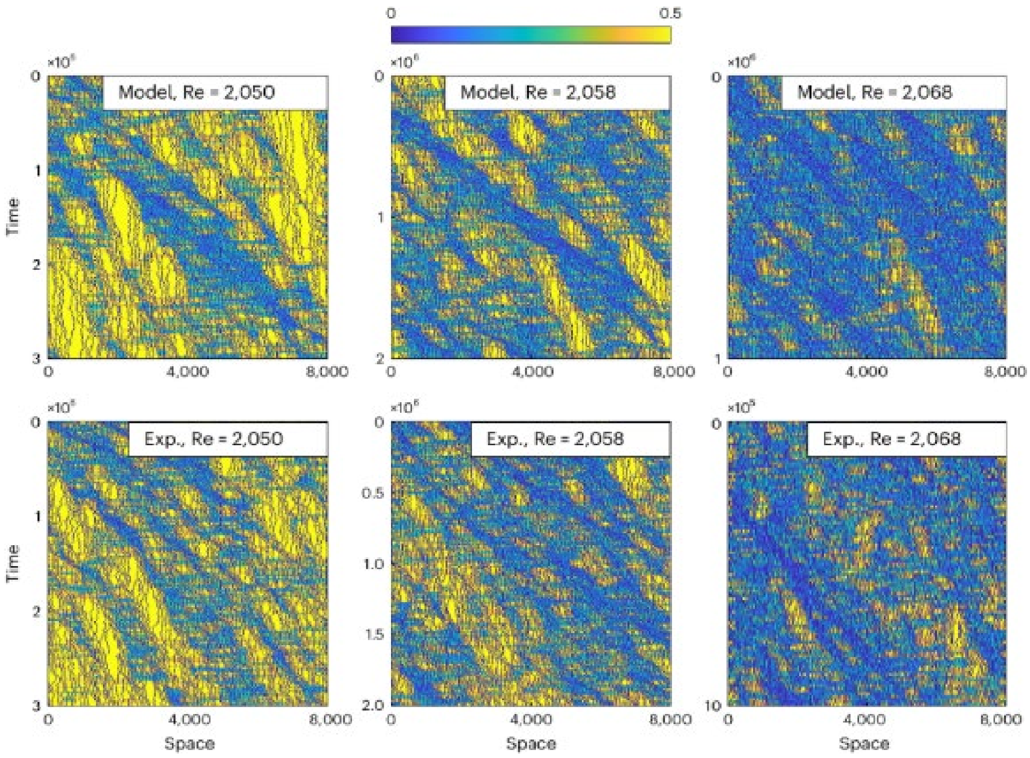


Fig. 1: Comparison of simulations of the continuous mesoscopic model for the multiple puff pipe flow and the experimental measurements [7].

Both theory and recent experiments in a quasi-one-dimensional Couette cell suggest that turbulence onset is a non-equilibrium phase transition in the directed percolation universality class [1-4]. Specifically, studies of statistical models with ecological interactions, based on simulations of hydrodynamic equations in pipe flow, show that the transition is governed by predator-prey dynamics between turbulence and an emergent large-scale flow, indicating a mathematical analogy between ecological extinction and turbulence decay [2]. Further studies on an extended model that includes energy input also explain the states away from criticality, showing how turbulent regions with expanding fronts develop as Re increases [5].

Recent experiments in pipe flow show distance-dependent repulsion between nearby turbulent puffs, leading to an unconventional jammed state not typically observed in directed percolation [6]. To investigate how general directed percolation is in transitional pipe flow, we developed both a stochastic coarse-grained model and a continuous dynamical model based on measured puff interaction functions. In line with renormalization group predictions, the numerical simulations of our models find strong evidence for critical scaling of the turbulent fraction in the directed percolation universality class, with a crystal-like spatiotemporal pattern arising from puff repulsion, as shown in Fig. 1. Our results indicate that the directed percolation transition is robust in pipe flow and independent of pairwise interactions in the multiple-puff scenario [7].

These studies on transitional turbulence demonstrate that the basic nature of the laminar-turbulent transition can be understood through statistical mechanics, and effective models capturing the coarse-grained dynamics of fluids provide a powerful tool for studying complex behaviors and predicting novel states in turbulent flows.

[1] M. Avila, D. Barkley and B. Hof, Annual Review of Fluid Mechanics 55, 575 (2023).
[2] H.-Y. Shih, T.-L. Hsieh and N. Goldenfeld. Nature Physics 12, 245 (2016).
[3] N. Goldenfeld and H.-Y. Shih. J. of Stat. Phys.167, 575 (2017).
[4] G. Lemoult et al., Nature Physics 12, 254 (2016).
[5] X. Wang, H.-Y. Shih and N. Goldenfeld, Phys. Rev. Lett. 129, 034501 (2022).
[6] V. Mukund. and B. Hof, Journal of Fluid Mechanics 839, 76 (2018).
[7] G. Lemoult et al., Nature Physics 20, 1339 (2024).

B. Reports of Postdocs

TG 1: Quantum Information and Quantum Computing

Jebarathinam Chellasamy (TG 1.1)

Jebarathinam explores quantum coherence as a basic feature of nonclassicality in foundations of quantum theory and quantum coherence as a resource in quantum information science.

In Jebarathinam et. al. [arXiv:2407.11755], the relationship between one-sided semi-device-independent steering and simultaneous correlations in complementary bases of quantum discord has been studied. This relationship operationally identifies information-theoretic characterization of the simultaneous correlations in more than one basis in quantum discord of two-qubit states. Quantum steering ellipsoid provides a faithful characterization of all forms of quantum correlations in two-qubit systems. This characterization has been invoked in the above research article.

In Jebarathinam et. al. [arXiv:2410.04430], the question of which aspect of bipartite coherence is essential to such semi-device-independent quantum information tasks going beyond standard Bell nonlocality or quantum steering is addressed. It has been shown that the global coherence of a single system can be transformed into bipartite entanglement. However, global coherence can also be present in quantum discord. At the same time, discord can display bipartite coherence locally, i.e., only in a subsystem or both subsystems. Thus, global coherence of bipartite separable states is defined here as a form of bipartite coherence that is not reducible to local coherence in any of the subsystems or both subsystems. To operationally identify such a notion of global coherence in discord, we demonstrate that global coherence is necessary to demonstrate semi-device-independent nonlocality of quantum discord in Bell or steering scenarios. From this result, it follows that any local operations that may create coherence locally are free operations in the resource theory of semi-device-independent nonlocality of discord. Applying this resource theory, it is identified that the quantum nonlocality beyond quantum steering acts as a resource for the quantum communication task of remote state preparation using two-qubit separable states. ■

Lee, Chen-Yu 李鎮宇 (TG 1.1)

Chen-Yu Lee proposed a novel approach for generating a squeezed laser applicable to both photons and phonons. Unlike conventional methods that employ $\chi^{(2)}$ nonlinear crystals to produce squeezed states, this innovative scheme utilizes red-sideband and blue-sideband transitions. This approach not only simplifies the experimental setup but also offers a versatile mechanism for achieving squeezing in both optical and mechanical systems. These advancements are significant for quantum technologies, where minimizing quantum noise is essential for enhancing the performance of quantum communication, precision measurement, and sensing applications.

In addition to the study of squeezed lasing, Chen-Yu Lee also investigated many-body localization (MBL) in disordered systems. The research focuses on how interactions in disordered environments lead to the suppression of quantum state diffusion, allowing for the preservation of localized states. This insight is crucial for developing strategies to maintain quantum coherence over extended timescales, which has significant implications for the development of quantum memory and resilience in quantum computing.

Wong, Renata (TG 1.1)

Since joining NCTS in November 2021, Renata Wong and her collaborators developed a quantum algorithm for protein structure prediction, with the respective paper published in [J. Parallel Distrib. Comput. 164: 178-190, 2022]. In another paper [IEEE Trans Nanobioscience 21(2): 286-293, 2022], she and coauthors designed a quantum way of inferring bits in unsorted databases which was inspired by methodology used in biomolecular algorithms. A quantum cryptographic protocol based on an algorithm for estimating simultaneously all mappings of a Boolean function using entanglement was proposed in [Quantum Studies: Mathematics and Foundations 10:1-13, 2023]. Her work on biomolecular and quantum algorithms for the independent set problem was published in [Scientific Reports 13, 2023], and a paper on quantum speedup for the maximum cut problem can be found in [IEEE Trans Nanobioscience 23(3): 499- 506, 2024]. She also has a chapter on quantum machine learning algorithms published in [Emerging Computing Paradigms, Wiley, ISBN: 9781119813408, 2022]. In the field of physics and philosophy of science, she and her collaborators worked on the issue of quantization of dynamics [J. Phys. Conf. Ser. 2197: 012027, 2022] and presented their in-depth analysis of problems facing current physical theories from the point of view of logic and philosophy of science [J. Phys. Conf. Ser. 2197: 012032, 2022].

Hsiao, I-Yun 蕭逸勻 (TG 1.2)

Hsiao I-Yun specializes in quantum control, focusing on developing efficient methods for superconducting qubit systems. In collaboration with Prof. Yen-Hsiang Lin from National Tsing Hua University and Prof. Yoshiaki Teranishi from National Yang Ming Chiao Tung University, this research aims to enhance quantum gate operations using nonadiabatic transitions.

The project utilizes nonadiabatic transitions in fluxonium qubits, demonstrating improvements in gate operation and qubit initialization. This method has proven to be more efficient than conventional approaches, showcasing its potential for practical quantum computing applications.

To advance towards real-world implementation, the team has investigated the impact of flux noise on gate stability, leading to a fast and robust design. Current efforts focus on analyzing decoherence effects to refine the method further, with the aim of aiding experimental groups in advancing superconducting qubit technology.

Shiau, Shiue-Yuan 蕭學遠 (TG 1.2)

Shiue-Yuan Shiau wrote a report on the physics of Frenkel excitons (60 pages), focusing on electron-hole pair exchange and many-body formalism (Annals of Physics, 458, 169431 (2023)). He studied the effect of the valence hole warping structure on exciton ground-state energy (Physical Review B 107, 235204 (2023)). In collaboration with experimentalists, he discovered a surprising photoluminescence signal made possible by the absorption of three photons in gold nanoparticles and WS2 monolayers (Cell Reports Phys. Science, 4, 101431 (2023)). He developed an ab initio quantum approach to electron-hole exchange for semiconductors hosting Wannier excitons (Phys. Rev. B 107, 115206 (2023)). He investigated the possible symmetry breaking for semiconductor excitons induced by Coulomb coupling between heavy and light holes (Phys. Rev. B 107, L081203 (2023)).

■

Kuo, En-Jui 郭恩瑞 (TG 1.3)

En-Jui Kuo has made notable contributions across several areas. In "Energy diffusion in weakly interacting chains with fermionic dissipation-assisted operator evolution" (Physical Review B 110 (7), 075149), he and his team explore energy transport in Majorana chains, revealing a diffusion coefficient scaling with interaction strength to the fourth power. Their work on "Training Classical Neural Networks by Quantum Machine Learning" (arXiv:2402.16465) proposes a method that reduces neural network parameters using quantum systems, showing practical effectiveness on standard datasets. In "Criticality-Ordered Recurrent Mean Field Ising Solver" (arXiv:2403.03391), Kuo's team introduces CoRMF, an efficient solver for Ising problems that improves accuracy and computational efficiency. His research with Nai-Hui Chia and Shih-Han Hung on "Oracle Separation between Noisy Quantum Polynomial Time and the Polynomial Hierarchy" (arXiv:2405.07137) demonstrates how noisy quantum circuits can surpass classical complexity classes. The "Quantum-Train" framework (arXiv:2405.11304), developed with a broad team including Hsi-Sheng Goan, addresses model compression in quantum-classical machine learning. Kuo's work with Jerry Yao-Chieh and others on "Computational Limits of Low-Rank Adaptation (LoRA) for Transformer-Based Models" (arXiv:2406.03136) analyzes the scalability limits of LoRA. Finally, his collaboration on "Self-Testing Quantum Error Correcting Codes: Analyzing Computational Hardness" (arXiv:2409.01987) advances the field of quantum error correction.

■

TG 2: High Energy Physics and Astrophysics

Beauchesne, Hugues (TG 2.1)

Weak supervision is a machine learning strategy that could be used at colliders to identify a signal within a background by directly training on the data. Even though extremely appealing, weak supervision searches suffer from the fact that neural networks require a large amount of data to learn a given task, greatly limiting the applicability of these searches. In [JHEP 02 (2024) 138], Hugues Beauchesne and his collaborators showed that techniques from transfer and meta-learning could be used to first train a neural network on a large set of potential models and then train on the actual data. The neural network then requires far less signal, thereby greatly improving the applicability of weak supervision searches. In [2401.03657 (accepted in EPJC)], the impact of deviations from the Maxwell-Boltzmann distribution on the abundance of dark matter in secluded sectors was studied. It was found that an abundance excess can appear at early times, but mostly vanishes because of a longer annihilation period. In [JHEP 06 (2024) 164] and [2407.01096], semi-annihilation of inert scalar multiplets was studied. It was shown that there does not exist any model of one multiplet for which semi-annihilation is efficient, but that certain models of two multiplets are viable. Furthermore, specific combinations of gauge numbers can lead to semi-annihilation being Sommerfeld suppressed, greatly relaxing indirect detection constraints.

■

García de la Vega, León M. (TG 2.1)

Leon M. Garcia de la Vega has studied the effect of a MeV scale gauge boson on Ultra High Energy neutrino - cosmic neutrino scattering (2406.19968 [hep-ph]). The main result of this work is to show that the possible resonant depletion of the UHE neutrinos observed in IceCube is already constrained by recent NA64 results and that in the near future this experiment will rule out this possible scenario - regardless of whether this MeV gauge boson measurably affects the magnetic moment of the muon or not. He has also studied a scenario where a spontaneously broken discrete symmetry, and not the continuous lepton number symmetry, mediates the Scotogenic Majorana neutrino mass generation mechanism (2407.14447 [hep-ph]). In this setup, which includes a dark matter candidate, a singlet scalar can mediate interactions between the visible and dark sectors, and the problem of introducing a Goldstone or gauge boson to the theory is avoided. Additionally, he and his collaborators in NCTS are studying a mechanism for generating Dirac neutrino masses with scalar leptoquarks, taking into account the possible effect of the right handed chirality of neutrinos on heavy meson decays. Finally, he and his collaborators in NCTS are studying the scalar sector of a dark Z model with a dark matter candidate, focusing on the interplay of dark sector observables and collider searches for new scalars.

■

Yamamoto, Yasuhiro 山本康裕 (TG 2.1)

Yasuhiro Yamamoto investigated light new boson signals in atomic physics and astrophysical observations. In atomic physics, he and his collaborators search for a light new boson effect as the violation of the King relation in precision isotope shifts. He had invented new analysis methods such as the generalized King relation, the dual King relation [Phys.Lett.B 838 (2023) 137682], etc. Some of them are the standard method to study the new physics search with isotope shifts. A novel method recently developed by him has been applied to new precise data of Yb isotope shifts measured by his collaborators of the quantum optics group in Kyoto University. They prepare a paper to show the new limit to the light new boson. He and his collaborator also studied these light boson signals with the stellar cooling. They pointed out that the stellar cooling constraints to the light new scalar boson were previously evaluated as a few orders of magnitude stronger than the actual constraints [Phys. Lett .B 843 (2023) 138027]. They also found that the large cancellation observed in these calculations does not occur when we include several couplings between the light scalar and the plasma components [arXiv:2407.17192[hep-ph]].

■

Ballav, Sourav (TG 2.2)

In collaboration with Prof. Wen-Yu Wen at Chung Yuan Christian University, they studied a four-qubit quantum circuit model of the evaporation of regular black holes. This model includes quantum gates that violates semi-causality by allowing transfer of information from inside the black hole to outside. They computed the corresponding von Neumann entanglement entropy and entanglement negativity of the Hawking pairs and found that quantum entanglement between Hawking pairs remain non-zero after the Page time, in contrary to the case when semi-causality holds. This work is in preparation.

■

Haldar, Parthiv (TG 2.2)

Dr. Parthiv Haldar analyzed aspects of quantum chaos in two different problems. In one he analyzed spectral complexity, a quantity introduced in the context of holographic quantum gravity, in the context of semiclassical quantum chaos. This provides an explicit calculation of the said quantity in the model of Riemann Zeta and modular billiard, which enabled explicit calculations using analytic and probabilistic number theory techniques. These calculations provide an explicit corroboration with expectations from Random matrix theory.

In a related work, Dr. Haldar applied the recently introduced scattering form factor in the context of the scattering theory of automorphic functions. In an ongoing work, Dr. Haldar analyzes resonances for scattering on congruence subgroups of the Modular group PSL(2, Z), in terms of non-trivial zeroes of Dirichlet L-functions with primitive characters. Under the assumption of the validity of the Generalized Riemann Hypothesis, the scattering form factor gives a novel way to connect the distribution of these zeroes to those of the eigenvalues of the Random matrices known as CUE, circular unitary ensembles. The work presents concrete numerical evidence for this connection. This work generalizes similar analysis for quantum scattering in Gurtzweiller's leaky torus model, where the corresponding resonances are explored in terms of non-trivial zeroes of the Riemann Zeta function. This work aims to analyze quantum arithmetic chaotic scattering with new quantities and explore further consequences. These works are being prepared and will soon be published.

■

Parihar, Himanshu (TG 2.2)

Himanshu Parihar studied the time-like entanglement entropy in a boundary conformal field theory (BCFT) from both field theory and holographic perspectives in a published work [JHEP 06 (2023) 173]. A novel Regge phase was observed which is distinct from space-like entanglement entropy phases and can have implications for emergent spacetime geometry from quantum entanglement. Subsequently, he with other collaborators explored the effect of backreaction on the entanglement entropy of Hawking radiation in a bath attached to a deformed eternal AdS black hole and its influence on the Page curve and mutual information [arXiv:2311.08186]. They find that backreaction delays the appearance of the island phase and shifts the Page curve with implications for Hawking radiation. They further investigated the reflected entropy in interface CFTs, analyzing phase structures and island contributions [JHEP 05 (2024) 143]. These results provide novel insights into the behavior of reflected entropy in systems involving AdS black holes and conformal interfaces.

Later they also introduced a massless Lifshitz scalar field theory in (1+1)-dimensions for an arbitrary anisotropy index *z* [JHEP 05 (2024) 284] and explored the z dependence of entanglement properties for the theory and proposed a z-dependent scaling for holographic entanglement entropy. In a follow up work [arXiv:2409.06667], they proposed a holographic duality for boundary Lifshitz field theory (BLFT) and derived g-theorems for two types of holographic BLFT, using both Neumann and conformal boundary conditions. They also computed the entanglement entropy holographically and observed that it agrees with the dual field theory results obtained using the path integral technique in the saddle point approximation.

In addition to the above work, they examined how the polarization degree of partially coherent light beams changes when propagating through Schwarzschild spacetime [Opt.Commun. 558 (2024) 130367]. This study provides a potential method for estimating the Schwarzschild radius of massive objects using optical polarization measurements.

■

Chan, Hei Yin Jowett 陳曦延 (TG 2.3)

Jowett Chan and his collaborators are involved in developing a local spectral scheme that was recently implemented into the fluid-wave hybrid scheme of the GAMER-2 code. This improves the numerical Schrödinger solver from a 6th-order to a 13th-order accurate scheme. Using the upgraded GAMER-2 code, we performed a self-consistent FDM cosmological zoom-in simulation of a Milky Way-sized halo containing substructures, which was not achievable by previous studies. Our simulation, conducted with a light particle mass of m=2×10^(23) eV, shows that the core structure and granulation of FDM subhaloes are more complex than those observed in simulated isolated haloes presented in previous studies. For subhaloes that survive, they do not follow the core mass-halo mass relation because the core mass remains intact while surrounded by granules of the host halo. For tidally disrupted subhaloe, core disruption occurs earlier than expected from previous works, which could be explained by the granules heating effect caused by the granules of the host halo. Our simulation serves as an important stepping stone toward FDM zoom-in simulations with larger particle mass. The above work will be split into two papers, one of which has been submitted to MNRAS.

■

Hsieh, He-Feng 謝和峯 (TG 2.3)

He-Feng Hsieh and his collaborators investigated gravitational wave emissions from rotating core-collapse supernovae. In addition to the previously known gravitational wave feature peaking at 400-500 Hz for slowly to rapidly rotating supernovae, they identified a new feature peaking at 1 kHz, observed exclusively in moderately rotating supernovae. Mode analysis confirms that both features are associated with the m=1 spiral deformation induced by the low-T/｜W｜ instability. However, the kHz feature is emitted from the inner proto-neutron star, while the sub-kHz feature originates from the outer region. Alongside the well-known bounce feature in rotating core-collapse supernovae, the newly identified kHz feature offers an additional diagnostic tool for estimating the angular momentum distribution within a collapsing core. This work has been published in ApJ, 961, 194 (2024).

■

On, Alvina Yee Lian 溫蕙蓮 (TG 2.3)

Alvina On joined NCTS in December 2022. She has been working with her collaborators on understanding the effects of radio depolarization in galaxy clusters. The fractional linear polarization is often used to constrain the intracluster magnetic field, which influences the formation and evolution of galaxy clusters. In On, Chan (Toronto), Lai (UCL) and Wu (UCL), they found that, in general, bright sources do not experience any significant changes in polarization, whereas faint sources either get severely depolarized or enhanced as their radiation propagates through the intracluster medium (PASA, under review). These effects should be considered when studying the magnetic fields using point source statistics in the field of a galaxy cluster. In a related work, Liou (NTHU), On and Yang (NTHU, Center Scientist) showed that different polarization signatures may arise from shock fronts and sloshing motions in a cluster merger simulation (MNRAS, in prep.). Magnetic fields also play an important role on smaller scales. During the 2023 NCTS-TCA Summer Student Program, On and her students analyzed the magnetic fields in interacting galaxies from their multi-wavelength emissions (ApJ, in prep.). One of her students Huynh (USTH, now KU Leuven) visited NTHU for three months under the 2024 NSTC International Internship Pilot Program. He successfully completed his BSc thesis with On and Pan (NTHU, TG Core) to study the impact of angular momentum and magnetic fields in core-collapse supernova simulations.

■

TG 3: Condensed Matter and Materials Physics

Kore, Ashish (TG 3.1)

Dr. Kore finished following work over the past year with Yang-hao Chan and Chi-Cheng Lee.

They conducted a detailed investigation into the origin of magnetism in the transition metal dichalcogenide (TMD) monolayer 1T-VSe2. Using first-principles-based density functional theory (DFT) calculations, they gained new insights into this fascinating material. They studied explicitly the prevailing notion that Stoner instability near the Fermi level is not the sole driver of ferromagnetism in 1T-VSe2. They also demonstrated that the magnetism in the monolayer can be precisely controlled by applying external strain. This allows the magnetic properties to be toggled on or off through strain-induced changes in the distance between neighbouring V atoms, the spacing between the two Se layers, and bond angles. This discovery opens up exciting possibilities for applications in spintronics and nano-electronics. Their findings reveal that structural distortions and atomic rearrangements play a crucial role in the emergence of ferromagnetism, highlighting the intricate interplay between electronic and structural factors. Finally, they explored the super-exchange interactions mediated through V-Se-V atoms, providing a compelling explanation for the observed relationship between structural changes and magnetism. These results deepen their understanding of the magnetic properties of the 1T-VSe2 monolayer and suggest new avenues for engineering magnetism in other TMDs.

■

Maghirang, Aniceto B., III (TG 3.1)

Aniceto B. Maghirang III is a collaborative and solutions-oriented researcher adept at using computer software focusing on materials modeling, data processing, and plotting in the field of Computational Quantum Materials. In particular, he employs

Density-Functional Theory with the help of the *Vienna Ab Initio Simulation Package* to probe the nontrivial topological properties and spin properties of two-dimensional (2D) materials. His primary approach is a high-throughput screening method to scan many 2D materials efficiently. His recent works (*Chinese Journal of Physics 86, 115-121* and *Chinese Journal of Physics 86, 242-254*) predicted the quantum Spin Hall effect in 2D half-Heusler and ilmenite oxide compounds and the Rashba effects on the latter. Specifically, 2D half-Heusler RbBeBi exhibited a system bandgap of 0.235 eV (with spin-orbit coupling) under the hybrid functionals while the nontrivial topologies persist even with crystal distortion, apparent in related half-Heusler compounds as well. Aside from this, he has started to use the popular open-source software Quantum ESPRESSO. Here, he focuses on studying the superconducting properties of materials by solving the isotropic Migdal-Eliashberg equations using the open-source F90/MPI code EPW by calculating the electron-phonon interactions and related materials properties employing Density-Functional Perturbation Theory and Maximally Localized Wannier Functions.

■

Sreeparvathy, Puthiya Covilakam (TG 3.1)

Sreeparvathy P. C. performed systematic first-principles calculations to identify the potential higher-order topological phase in a few antiperovskite materials [New Journal of Physics 26 (7), 073007 (2024)]. Notably, all the investigated materials exhibit multi-Dirac states near the Fermi level. Moreover, she examined the higher-order topological properties using Z_4 topological number and hinge state calculations. In addition to the antiperovskite materials, she was also involved in the detailed study of quantum spin Hall states in two-dimensional MA_2Z_4 materials $SrTl_2Te_4$ and $BaTl_2Te_4$ [Applied Physics Letters 124 (23), 233102 (2024)]. In this work, they examined the electronic structure, Z_2 topological invariant and potential edge states of these materials. In addition, they investigated the role of electric fields and strains on the topological properties. In the third project, Sreeparvathy and her collaborators studied the higher fold topological phonon and electron states in cubic chiral materials. This study discussed the spin-1 Weyl and charge-2 Dirac topological phonon states in the phonon spectrum of a few ternary materials. In addition, they have examined the higher-fold electronic states near the Fermi level. For the fourth project, she and her collaborators focused on fertile Dirac states in the bulk PbFCl type materials. Moreover, she performed a detailed study of graphene-based two-dimensional systems, which allow the coexistence of the higher-order corner modes and Weyl phonons.

■

Remund, Kimberly (TG 3.2)

Kimberly Remund and her collaborators' research interests are centred on the mysterious Planckian strange metal phase, characterized by a perfect linear temperature dependance of the resistivity, a universal linear temperature dependent scattering rate and a logarithmic temperature dependance of the specific heat, which phase has been observed in high-Tc cuprate superconductors near optimal doping. In their recent work, they proposed a microscopic mechanism based on a heavy-fermion approach of the slave-boson t-J model. They showed that via controlled perturbative renormalization group analysis, over a finite range in doping, a quantum critical phase exhibiting Planckian scattering rate was found [Y.-Y. Chan, K. V. Nguyen, K. Remund, and Chung-Hou Chung, arXiv2406.14858]. Following on their previous results, they computed the charge susceptibility allowing them to access correlations of electron density fluctuations within the Planckian metal phase of their model. Anomalous (momentum-independent) density fluctuations have been reported in cuprates within the strange metal phase by M-EELS technique, and yet not been explained by existing models. In their most recent work, they show that their results offer an excellent description of anomalous (momentum-independent) density fluctuations as seen in experiments [K. Remund K. V. Nguyen, and Chung-Hou Chung., in preparation].

Her research work has also been focused on the physics of multi-polar spin systems and more particularly spin-1 magnets. They used a formalism based on the u(3) algebra which allows dipole and quadrupole moments to be treated on an equal footing. Their work on spin-1 systems and pioneering application of the u(3) formalism to dynamics and thermodynamics of magnets largely contributes to the development and understanding of spin-1 systems [K. Remund et al., Phys. Rev, Research 4 033106 (2022); K. Remund et al., in preparation]. They also generalized the u(3) formalism to the description of classical spin-1 within a Self-Consistent Gaussian Approximation (SCGA) scheme in order to properly access classical dipolar and quadrupolar correlations even in disorder spin-1 systems, such as spin-liquids [K. Remund et al., in preparation].

■

Tzeng, Yu-Chin 曾郁欽 (TG 3.2)

Yu-Chin Tzeng extended the concept of fidelity susceptibility from Hermitian quantum systems to non-Hermitian systems [Phys. Rev. Research **3**, 013015 (2021)]. Their definition of fidelity preserves several general properties and has been adapted in numerous non-Hermitian systems to effectively detect exceptional points [Quantum **7**, 960 (2023)]. Additionally, Yu-Chin has investigated quantum entanglement in non-Hermitian systems, introducing generic von Neumann and Rényi entanglement entropies for these systems. These entanglement measures capture the essential physics of non-Hermitian many-body systems and effectively reveal the negative central charge in non-Hermitian critical systems through logarithmic scaling. Known as the Tu-Tzeng-Chang entanglement entropies, these measures are now widely used to study non-Hermitian critical systems [SciPost Phys. **12**, 194 (2022)]. Building on this line of research, Yu-Chin analytically investigated the entanglement Hamiltonian and entanglement energy spectrum of a non-Hermitian spin ladder using perturbation theory in the biorthogonal basis. They found that, for the maximally entangled ground state, the entanglement Hamiltonian closely resembles the subsystem Hamiltonian, albeit with renormalized coupling strengths, enabling the definition of an effective temperature. This discovery provides new insights into quantum entanglement in non-

Hermitian systems and lays the groundwork for novel approaches to studying finite-temperature properties in non-Hermitian quantum many-body systems. [SciPost Phys. Core (2024) to be published] In addition to his work on non-Hermitian systems, Yu-Chin has contributed significantly to Hermitian quantum many-body physics by exploring quantum phase transitions via energy cross-derivatives [New J. Phys. **25**, 043006 (2023)] and identifying a novel quantum phase transition from a metal to a topological insulator, particularly at 1/4 electron filling under strong correlation effects. [Phys. Rev. B **107**, 155106 (2023)]

■

TG 4: Interdisciplinary Research

Fukusumi, Yoshiki 福住吉喜 (TG 4.1)

Yoshiki Fukusumi has proposed a new canonical way to study group extension of chiral conformal field theories in [arXiv:2405.05178]. The group extension of chiral conformal field theories is the building block of topologically ordered systems in condensed matter but they are outside of existing frameworks, modular tensor categories. However, only by assuming established data of full conformal field theories, a series of chiral conformal field theories can be obtained from his formalism. Moreover, by revisiting the classification of conformal field theories in [arXiv:2408.04451], he has demonstrated physics of edge modes in topologically ordered systems has been governed by emergent integrable renormalization group flows. The nonlinear version of chiral Luttinger liquid which may be realizable is a typical example, and the new framework is one of the most reasonable generalizations of existing theoretical studies.

■

Chen, Wei-Chih 陳威智 (TG 4.2)

Wei-Chih Chen collaborated with the experimental chemists to explore the mechanical selectivity of Hirao coupling, a palladium-catalyzed cross-coupling reaction forming phosphonates from dialkyl phosphites and aryl halides. The new heteroleptic palladium precatalysts demonstrate high catalytic efficiency in cross-coupling such response. He uses DFT calculations to study the reductive elimination mechanism in this reaction. This study investigates the role of steric effects in Hirao coupling using palladium complexes with secondary phosphine oxides-based ligands. Computational analysis reveals that bulkier ligands increase the reaction barrier during reductive elimination, resulting in lower yields. Conversely, less bulky ligands enhance product yield, aligning with experimental observations on chemical selectivity. (*Dalton Trans.*, 2023, **52**, 5101-5109.)

■

Goswami, Koushik (TG 4.3)

Koushik Goswami and his collaborators at the National Center for Theoretical Sciences investigate the conformational and dynamical properties of partially active polymers in the context of chromatin modeling. Inspired by the nonuniform activity observed along chromatin due to varying motor activity and ATP consumption rate, they model the polymer as a chain with an active segment of tunable size and location. Notably, they find that even with fixed activity, the placement of the active segment significantly influences the polymer's conformation. For example, positioning the active segment at the chain's end enhances swelling compared to placing it centrally. This effect is also reflected in the dynamics, where a tagged point within the active region displays enhanced superdiffusion and more pronounced subdiffusion. These results are compiled in a manuscript that is ready for submission to a scientific journal.

Additionally, Goswami studies stochastic resetting of a tracer in a nonequilibrium bath, where bath particles interact harmonically with the tracer and exhibit differing diffusivities (or temperatures). This model closely relates to probe motion in an active viscoelastic medium, as exemplified by membrane fluctuations of the nucleus controlled by cytoskeletal and chromatin activity. He demonstrates that, depending on the diffusivities of the bath particles, interactions can either facilitate or hinder the tracer's search for a target at an optimal resetting rate. This work has been submitted to a scientific journal.

Goswami and his collaborators at the University of Potsdam published a paper on the anomalous diffusion of active tracers in gel networks in *Physical Review E*, **110**, 044609 (2024).

■

Wu, Chia-Chou 吳嘉洲 (TG 4.3)

At NCTS, my research focuses on the mechanisms of large-scale, coordinated cell death and its roles in development and disease and was published (*Nature* **631**, 654–662 (2024)). We have identified that ferroptosis—an iron-dependent form of cell death—propagates across tissues through "trigger waves" of reactive oxygen species (ROS). Unlike diffusion-limited processes, these waves travel at constant speeds over long distances, allowing localized death signals to amplify into widespread cellular destruction.

Our work demonstrates that ROS feedback loops, including the Fenton reaction, NADPH oxidase signaling, and glutathione synthesis, are critical for sustaining these waves. Under ferroptotic stress, cellular redox systems shift from monostable to bistable states, enabling cell populations to support self-propagating ROS waves. This bistability transforms affected cells into a medium that consistently transmits ROS and lipid peroxidation products.

These findings were validated by studying ferroptosis in avian limb muscle development, where precise cell death events facilitate muscle differentiation and segmentation.

Occurring in spatially restricted zones, ferroptosis sculpts muscle structure and exemplifies how large-scale cell death mechanisms operate in vertebrate morphogenesis.

This research deepens our understanding of cell death coordination beyond apoptosis, positioning ferroptosis as a major driver of large-scale cell death in both normal development and disease contexts. By uncovering the role of ROS feedback and redox bistability, our findings offer new therapeutic strategies for managing pathological cell death in degenerative diseases.

■

IV. On The NCTS Physics International Advisory Committee Meeting, June 20-21, 2023

Phase V of the NCTS started from Jan. 1, 2021, and thus we are nearly at the end of the first half of the third year of Phase V. The main purpose of this on-site IAC Meeting is to invite the IAC members to provide comments on the operations and achievements of the Physics Division in the past two and half years, to offer recommendations and suggestions on how to better achieve the goals of the NCTS.

We are rather fortunate that the following five members of the IAC were able to participate the IAC meeting last June: Profs. Eberhard K. U. Gross (Hebrew University of Jerusalem, Israel); Jean-Francois Joanny (PSL Research University, Paris, France); Kimyeong Lee (Korea Institute for Advanced Study, Seoul, Korea); Chung-Pei Ma (University of California, Berkeley, USA), Naoto Nagaosa (RIKEN, Saitama, Japan).

During the two-days meeting of the busy Program (see Appendix A below), the IAC members worked very diligently and efficiently. They listened to the opening address by NTU Executive Vice President Wanjiun Liao, reports from the Directors and Thematic Group (TG) Coordinators, talked to some EC Members, Center Scientists and Center Postdocs, and also toured the Center viewing the Center facilities etc. They helped us to identify problems and to give comments and suggestions to improve the Center to a higher level of excellence. We are very grateful to our IAC members. The report of recommendations by the IAC is enclosed in Appendix B at the end of this Report. We have been working on implementing recommendations by the IAC Members.

Photo 1 First row from left to right: Wanjiun Liao (NTU VP), Chung-Pei Ma (IAC), Eberhard Gross (IAC), Jean-Francois Joanny (IAC), Kimyeong Lee (IAC), Naoto Nagaosa (IAC).

A. The IAC Meeting Program

Time	Item / People	Place / Notes
June 20, 2023 (Tuesday)		
09:20-09:30	Opening Address: Executive Vice President Wanjiun Liao	4th Floor Lecture Hall
09:30-10:30	Report of the Director: Guang-Yu Guo (NTU)	4th Floor Lecture Hall Chair: Jeng-Da Chai (NTU)
10:30-11:00	Coffee Break	Outside Lecture Hall
11:00-11:30	Report of Thematic Group 1.1: Hsi-Sheng Goan (NTU)	4th Floor Lecture Hall Chair: Jeng-Da Chai (NTU)
11:30-12:00	Report of Thematic Group 1.2: Ray-Kuang Lee (NTHU)	
12:00-12:10	Site Introduction: Guang-Yu Guo (NTU)	
12:10-12:20	Group Photo	In front of the Entrance
12:20-12:30	Tour of the Center by IAC Members	
12:30-13:30	Lunch Break	7th Floor Lounge
13:30-14:00	Report of Thematic Group 1.3: Hong-Bin Chen (NCKU)	4th Floor Lecture Hall Chair: Jeng-Da Chai (NTU)
14:00-14:30	Report of Thematic Group 2.1: Cheng-Wei Chiang (NTU)	Chair: Henry Tsz-King Wong
14:30-15:00	Report of Thematic Group 2.2: Yu-tin Huang (NTU)	
15:00-15:30	Report of Thematic Group 2.3: Min-Kai Lin (IAA-AS)	
15:30-16:00	Coffee Break	Outside Lecture Hall
16:00-16:30	IAC meets TG1-2 Coordinators + EC Members	4th Floor Lecture Hall
16:30-17:00	IAC meeting: Prepares comments and recommendations	Meeting Room 429
18:30	Dinner with TG Coordinators + EC Members + Hub PI's	水源會館
June 21, 2023 (Wednesday)		
09:00-09:30	Report of Thematic Group 4.1: Pochung Chen (NTHU)	4th Floor Lecture Hall Chair: Jeng-Da Chai (NTU)
09:30-10:00	Report of Thematic Group 4.2: Liang-Yan Hsu (AS)	
10:00-10:30	Report of Thematic Group 4.3: Pik-Yin Lai (NCU)	
10:30-11:00	Coffee Break	Outside Lecture Hall
11:00-11:30	Report of Thematic Group 3.1: Feng-Chuan Chuang (NSYSU)	4th Floor Lecture Hall Chair: Guang-Yu Guo
11:30-12:00	Report of Thematic Group 3.2: Chung-Hou Chung (NYCU)	
12:00-13:00	Lunch Break	Room 429 / Lecture Hall
13:00-13:40	IAC Meets Hub PI's and TG3-4 Coordinators	4th Floor Lecture Hall
13:40-14:40	IAC Meets NCTS CSs	Lecture Hall
14:40-15:30	IAC meets NCTS postdocs	Lecture Hall
15:30-16:00	Coffee Break	Outside Lecture Hall
16:00-16:30	IAC meets Director and Deputy Director (Asks questions and clarifications)	Meeting Room 429
16:30-17:00	IAC meeting: Prepares comments, recommendations and outline the IAC report	Meeting Room 429
17:00	Close	

B. Report of the International Advisory Committee

Five members of the International Advisory Committee, Profs. Eberhard Gross, Jean-Francois Joanny, Kimyeong Lee, Chung-Pei Ma and Naoto Nagaosa, participated the in-person IAC Meeting on June 20-21, 2023. After listening to the presentations by the NCTS Physics Division Director and Thematic Group Coordinators, and extensive discussions with the Center Scientists and members of Center Research Staff, we would like to provide the following report for record.

I. On the organization, Program and Personnel

Even though it is not a "one-roof" center and "soft", it is functioning quite well producing many important outputs and outcomes. It is made from the headquarters at NTU and 4 Hubs distributed over Taiwan, but the communications among the members are performed effectively. The structure of the center is well organized. The important decisions can be made efficiently and effectively in a democratic way.

We are told that the major program of the Physics Division currently is the Thematic Group (TG) Program. Eleven TGs were established in Jan. 2021, based on two considerations: (1) teams in Taiwan that are internationally competitive in fields that are important in the coming decade and (2) fields that are important for the next decade and Taiwan has the potential to do well with sufficient support or cannot afford to be left out. TGs and their associated Center Scientists (CS) are reviewed every two years. Thus, the present 11 TGs were reviewed and approved by the Executive Committee at the end of 2022.

We all agree that the activities of the center are very well organized and functioning efficiently producing many important scientific outputs. Every TG is organizing many conferences, meetings and schools promoting collaborations within Taiwan and internationally, and we highly evaluate their serious efforts including the strong leadership of the center director. The evaluation of Center Scientists (CSs) every two years requires huge effort of both Executive Committee and members of center, and we suggest to consider the possibility to extend the interval between the evaluations, e.g., 5 years. This is closely linked to the term of the postdoctoral (PD) positions. Usually, 2 years PD position is less appealing for the candidates and we are afraid that the good people will find another better offer.

Incentives for the CSs is also important. The additional compensation (salary) for them is too small from the international standard and we suggest to increase its amount. We regard additional 20% to the main salary is the reasonable amount. It is a highly effective investment considering the size of the research budget. Also, more support from each university or institute by, e.g., reducing the teaching or administrative burden for the CS, is recommended.

We are also aware that the NCTS is a soft center. Its Physics Division currently have 30 Center scientists (CSs) who are outstanding scholars from various institutions in Taiwan. Roughly, there are 3 CSs in each TG, who together with the associated core members, run the respective TG. Roughly, about 4 M budget is allocated to each TG which can be used to hire postdocs and organize activities, such as conferences, schools and hands-on courses etc.

We understand that each CS of NCTS has his/her sources of research grant and PDs besides those from center, and 4M is not the whole budget he/she can use. However, it is desirable to increase this amount, since it is the most efficient investment considering the present activity of the center. Most important concern is the support from the National Science and Technology Counsel (NSTC), which is connected to the matching grant and hence should be stable or increased. Otherwise, it is difficult for NCTS to make long-term plan, and also offer a reasonable length for the PD position. Especially, the budget cut due to the pandemic should be recovered to (or even more increased from) that before COVD-19 since all the activities are now back to normal state now.

We learn that 26 postdocs and 7 research assistants worked here in the first 5 months this year. Currently, there are 3 research assistants and 22 postdocs (9 Taiwanese; 8 Indians; 2 Canadian; 1 Japanese; 1 Polish; 1 Filipino; 1 Brunei; 1 Slovak; 1 Colombian). The research staffs including PDs are at the very high level as evidenced by the impact of published papers and several awards including international ones. There produce many papers in high profile journals. This indicates that the center occupies an important position internationally, and leading the researches of theoretical physics in Taiwan. The ratio of domestic people is less than half, and the center is already international.

It is most important that the researchers in NCTS can have enough time to devote to research not disturbed by administrative works etc. The efficient operation of the center is highly desired.

II. On the academic activities and achievements

We learn that one of the goals of phase V of the NCTS is to become a center of excellence. In this respect, we notice that even though the size of the center is not so large, e.g., compared with APCTP in Korea, in spite of the smaller budget and number of people, the productivity is comparable both qualities and quantities. Here we list highlights of the important achievements from each TG.

TG1.1 addresses one of the most important and most promising applications of quantum computing namely the prototypical problem of electronic structure theory where the time cost of computing the eigenvalues and eigenfunctions of the time-independent many-electron Hamiltonian scales exponentially with system size using classical computing. Quantum computing holds the promise of polynomial scaling which, in principle, can be achieved by encoding a fermionic system of N spin orbitals into a system of qubits. For reasons of decoherence and other technical constraints, the number of qubits required in this encoding should be as small as possible. The authors propose a systematic and very efficient encoding scheme where the number of required qubits has an upper bound of O(mxlogN) where m is the number of particles. The power of the method is successfully demonstrated for the H2 and the LiH molecules where the number of required qubits is significantly lower than for standard encoding schemes (Phys. Rev. Research 4, 023154 (2022)).

TG1.2 is working on the quantum physics and quantum engineering, especially on the platform of quantum computing such as superconducting qubit, trapped ions, and photonic systems. An impressive work by this group is the application of the machine learning technique to extract the degradation quantum information in squeezed state, where a fast, robust, and precise quantum state tomography for continuous variables has been demonstrated. [Phys. Rev. Lett. 128, 073604 (2022)]

TG 1.3 addressed several important questions in quantum information science, including this one: can a collection of marginal information reveal additional new marginal information? They answer this affirmatively and show that (non-) entangled marginal states may exhibit (meta)transitivity of entanglement [npj Quantum Information 8, 98 (2022)].

TG2.1 developed an efficient numerical simulation code for modelling the neutrino transport including collisions and their flavor oscillations in multiple dimensions. In a work (Phys.Rev.Lett.130(1023)11), Dr. Meng-Ru Wu in collaboration with colleagues in Taiwan has proposed a novel way to probe interaction between light dark matter and standard model particles by utilizing supernova neutrinos. Dr. Meng-Ru Wu won 2022 AAPPS-APCTP CN Yang Award for his excellent work in this topic.

TG2.2 developed, by Dr. Yu-Tin Huang in collaboration with colleagues in IAS and UCSB, a relation between causality, unitarity and the weak gravity conjecture in the study of charge-mass ratio of extremal black holes. In this work (JHEP03(2022)083), the additional implication of the effective field theory with UV completion in quantum gravity and the swampland conjecture has been studied. Dr. Yu-Tin Huang is an international leader in the study of scattering amplitude and its relation to gauge theories and gravity. He got a 2020 OCPA award.

TG 2.3 (theoretical and computational astrophysics) was established in Phase V of NCTS and is the newest group of the center. Leaders of this group have included capable young astrophysicists such as center scientists Min-Kai Lin, Hsiang-Yi Yang, Hsi-Yu Schive, and Yueh-Ning Lee. The group's research portfolio is broad, spanning theories and simulations of planet and star formation, to studies of the nature of dark matter and large scale properties of galaxies such as the so-called Fermi bubbles in the Milky Way (Yang et al 2022). The outreach effort in running the undergraduate summer student program is commendable. The gender diversity of this group is exemplary and should be emulated by other TGs.

On TG3.1, in a very fruitful and highly productive collaboration of NCTS researchers with the group of Prof. Steven G. Louie at UC Berkeley, several important aspects of exciton-phonon coupling were investigated, fully ab-initio, in second-order perturbation theory where photon and phonon are treated on equal footing. In monolayer MoS2, the internal spin-structure of the excitons is found to be crucial in the prediction of an unexpectedly long lifetime of the lowest-energy bright A exciton (Nano Lett. 23, 3971 (2023)).

TG3.2 studied, in collaboration with the experimental group, the quantum critical phenomenon of heavy fermion system to reveal the microscopic mechanism of the Planckian dissipation appearing in the resistivity. ("The scaled-invariant Planckian metal and quantum criticality in Ce1−xNdxCoIn5", Nature Communications 14, 581 (2023)).

TG4.1 studied asymmetric junction between the two 1D interacting electron systems by combining analytic method (bosonization) and numerical method (infinite matrix product state (iMPS)) to obtain a reasonable agreement between the two. Especially, it is remarkable that they can treat the infinite systems numerically. [“Two-wire junction of inequivalent Tomonaga-Luttinger liquids”, Phys. Rev. B104, 235142 (2021)]

TG4.2 studied the skin cells which undergo asynthetic fission to expand body surfaces in zebrafish (K.Y. Chan et al. Nature 605, 119-125 (2022)). During development, the area of a growing animal increase and the skin must adjust to insure proper epithelial coverage. Together with biology groups, C-P Hsu show, on experiments on zebrafish, in this work that this is partly done by a new and original type of cell division that they call asynthetic fission. They show very convincingly that during these divisions there is no DNA replication and that the produced cells have a reduced genome size.

TG4.3 has a very broad spectrum going from physical-chemistry, soft condensed matter, colloïdal systems, food physics, active matter to the physics of biological systems, evolution and ecology and more fundamental physics questions such as stochastic thermodynamics, turbulence and non-equilibrium statistical mechanics. The group is somehow singular at NCTS since it includes two experimental teams and it is one of the groups where collaborations with experiments are the strongest, with external experimental physicists but also with physico-chemists and several biologists in Taiwan at the Institute of Molecular Biology and at the Institute of Bioinformatics and Systems biology. One should note also that several theory groups started their own experimental activities. This certainly gives this thematic group a very interdisciplinary character, which is one of its strengths. The papers published by the group are published in physics journals but also in biology journals sometimes very high profile (Nature group or eLife).

Despite the broad diversity of subjects studied among the members several unifying themes appear. A clear one is non-equilibrium statistical physics that has fundamental aspects such as the study of the efficiency of active engines or some non-equilibrium models of aggregation but also more "applied" aspects for the study of some biological or biomimetic systems. Statistical physics is less present in other TGs and the group is involved in several schools and workshops in statistical physics in Taiwan but more broadly in east Asia. Another strongly unifying theme is the fact that many of the problems studied are either coming from biology (equilibrium and nonequilibrium membranes for example) or inspired by biology (and therefore raise more general questions in non-equilibrium statistical physics). Finally, numerical simulations are a tool extensively used throughout the group.

Many of the questions raised by this group are extremely timely and in some cases hot topics to which important contributions have been made. This is the case of the work on turbulence inspired by the recent work of N. Goldenfeld or the work on local phase separation in cells which is proposed as a highlight of TG4.3. Some of the problems studied are also very original such as the rheological study of aiyu which is a popular summer dessert and which raises interesting questions associated to the gelation phenomenon. Finally, the group is well organized and fully plays its role in organizing conferences and workshops and in trying to promote mentor younger scientists. It currently hosts one research fellow and one postdoc. The group has been existing for many years and the older scientists who run it would like to leave the leadership to younger scientists. This should not be a problem, considering the high level of the younger scientists whom we met.

Highlight: (Enhanced DNA repair through droplet formation and p53 oscillations M.S.Heltberg et al. Cell 185, 4394-4408 (2022)). This works by the group of SH Chen and a biology groups. The theoretical part of the work presents a model for the formation of foci where in which the DNA repair machinery can be embedded due to local condensation. The observed oscillations of the protein p53 are shown to be coupled to the growth of the foci and to limit the associated Ostwald ripening.

We notice that another goal of the NCTS is to cultivate young theoretical scholars. The Division typically organizes a dozen of summer/winter schools and hands-on courses. The division has also allocated a significant percentage of the funding to support its postdocs as well as students to attend international conferences. The division has also set up three annual awards to encourage researchers to do high quality research in theoretical physics.

The efforts to cultivate young people are highly appreciated, and its achievements are well recognized. For example, Dr. Meng-Ru Wu (ASIoP) was awarded the 11th C.N. Yang Award. We also note that three previous PDs of members of TG1.3 have successfully obtained faculty positions in Taiwan: Prof. Chia-Yi Ju at NSYSU since 2022, Prof. Shin-Liang Chen at NCHU, and Huan-Yu Ku at NTNU since Aug. 2023. Compared to other TGs, this demonstrates the remarkable ability of TG1.3 to cultivate young theoretical scholars and launch their academic careers.

NCTS organizes many schools and courses, and send the young students and PDs to international conferences. It is also an excellent idea to give three awards to young people, which should be continued. We do not criticize, but are afraid that organizing so many meetings put the heavy burden for the CSs and reduces their time and energy for their own researches. We regard that the efforts are far more than enough, and can be reduced if they want. Instead, we suggest to trigger the organization of inter-TG seminar or workshop by the PDs to promote their interaction.

The Division has not done enough in promoting gender diversity and cultivating careers of female theorists. See last comment in Sec III.

We are aware that another goal of the NCTS is to enhance the extent and breadth of interdisciplinary researches as well as the collaboration with experimentalists. Indeed, the 11 TGs were grouped into 4 grand TGs, which were designed to provide platforms for bottom-up collaborations among the regular TGs within it. The collaborations among the TGs are functioning within TG1, and can be extended to other TGs also. For that, we suggest the following two themes, which are relevant to many TGs. One is the machine leaning and AI. This method is now employed in many branches of physics including both theory and experiment. The development of this method as well as its applications can be the theme of inter TG collaborations. The other is the decoherence problem, which is crucial for the quantum information technology, quantum chemistry, and condensed matter physics. To reveal its microscopic mechanism and predict its magnitude is an important theoretical goal, which can be tackled by the collaboration among TGs.

We can see that the collaborations between theory and experiment are already going on in e.g. TG1.2, TG2.1, TG2.3, TG3.1, TG3.2, TG4.3, producing important research products. To further promote the collaboration among TGs and also with other institutions in Taiwan, we suggest the monthly or bi-monthly Colloquium series by the CSs in hybrid form, which introduces the research topics in a pedagogical way. This will be also useful to inspire the young people.

We learn that the last major goal of the NCTS is to serve as an efficacious channel to network the home researchers with other scholars and preeminent overseas institutions. Indeed, we see that the collaborations with oversea researchers are everyday occurrence in NCTS. Organizing many conferences and workshops, and inviting distinguished scholars, the center forms the effective world-wide networks. Setting up MOU with 14 institutions in East Asia, India, Europe, Australia, and US, NCTS forms an international network of collaborations. Sending PDs to international conferences is another effective effort to form the network.

Although each TG has produced many important scientific products, it is desirable to promote the collaboration among TGs more. For example, is it possible to have an annual in-person meeting where all the members get together?

III. On the Center's environment and resources

The NCTS is at the center of Taipei and convenient from airport and public transportation. It is surrounded by many departments and institutes, which facilitates the interdisciplinary collaborations. The headquarter in Chee-Chung Leung Cosmology Building of NTU also offers an ideal platform for the theoretical studies. The physics department, mathematics department including Academica Sinica Mathematics, and astronomy department of NTU are located on neighboring buildings.

The 4th floor of Chee-Chung Leung Cosmology Building on the NTU Campus is borrowed from the Department of Physics, NTU, and shared with Math. Division with free charge. The 3rd floor is rented with rather high cost. They have 21 offices, 1 Lecture Hall, 1 Seminar Room, 1 Meeting Room, and Lounges/Coffee Rooms. Sharing each office by two scholars, they have enough space to accommodate the visitors. The administrative staffs are extremely efficient and functioning well. Numerical calculations are performed mostly on supercomputers in National Center for High-performance Computing, while they also have the inhouse Computing Server with CPU and GPU nodes.

We recognize that the National Science and Technology Council (NSTC) is the main funding agency of the NCTS. The Physics Division receives roughly up to 40 M NTD/year from the NSTC. The hosting NTU provide a matching fund of 40 % of what they receive from the NSTC. Thus, the Division receives in total about 56 M NTD/year. As mentioned above, NCTS is producing scientific output with extremely high efficiency considering its budget size. Although each CS has his/her own budget besides that from the NSTC, it is evident that the increase of funding will definitely increase the scientific product even more. The decrease or the unstable funding from the NCTS results in decrease of the matching fund, and can be a fatal damage for the center. This is because the fundamental cost such as the employment cost cannot be reduced, and hence the budget for the research activities is mostly affected by this budget cut. This is also linked to the term of the PD hiring.

We recognize that the hosting university NTU supports NCTS very well. For example, NCTS can use the 4th floor of Chee-Chung Leung Cosmology Building for free. It would be even more helpful that the burden of CSs can be reduced in number of classes or other administrative duties.

We believe the Division’s resources are utilized quite efficiently. We appreciate very much the devoted effort by director and deputy director to run the center. We do not have any complain.

We encourage NCTS to reflect on the lack of gender balance and create plans to improve the situation. We note that all 11 TG speakers were male, and some TGs had no women on the roster. Beyond head counts, NCTS should take leadership in identifying and addressing potential problems in research climate for women and under-represented minorities. While gender diversity is a serious problem in theoretical physics worldwide, NCTS appears to be behind other top research centers in its awareness of and efforts to address the issue.

Naoto Nagaosa

Prof. Dr. Naoto Nagaosa

On behalf of the five participating IAC Members

2023-2024 NCTS PHYSICS

Biannual Report

National Center for Theoretical Sciences - Physics Division

4th Floor, NTU Cosmology Hall

No. 1, Sec. 4, Roosevelt Rd., Taipei 106319, Taiwan

https://phys.ncts.ntu.edu.tw