

## NCTS Theoretical Physics Symposium 理論物理論壇

(2022/1/25)

**Morning session 9:00 – 10:30**

**Chair: Feng-Chuan Chuang (NSYSU)**

**Location: 理學院大樓 E101 College of Science Building E101**

No.	Time	Name	Title of talk
1	9:00 – 9:30	Min-Kai Lin (IAA-AS)	Modern challenges and hopes for planet formation
2	9:30 – 9:50	Jeng-Da Chai (NTU)	TAO-DFT and Its Applications to Nanomaterials with Radical Nature
3	9:50-10:10	Jhih-Shih You (NTNU)	Supermetal-insulator transition in a non-Hermitian network model
4	10:10-10:30	Guang-Yu Guo (NTU)	Introduction to NCTS-Physics

**Afternoon session 13:30 – 15:00**

**Chair: Guang-Yu Guo (NTU)**

**Location: 理學院大樓 E101 College of Science Building E101**

No.	Time	Name	Title of talk
5	13:30 – 14:00	Yu-tin Huang (NTU)	The gravitational S-matrix
6	14:00 – 14:20	Meng-Ru Wu (IOP-AS)	Supernovae as astrophysical laboratories for fundamental physics
7	14:20 – 14:40	Yueh-Nan Chen (NCKU)	Performance of quantum state transfer on IBM-Q, Ion-Q, and QuTech devices
8	14:40 – 15:00	Yang-Hao Chan (IAMS-AS)	Exciton-phonon dephasing and linewidth from first-principles in monolayer MoS <sub>2</sub>

[1]

### **Modern challenges and hopes for planet formation**

Min-Kai Lin

Institute of Astronomy and Astrophysics, Academia Sinica, Taipei 10617, Taiwan

Abstract: Planet formation appears ubiquitous in the universe. However, the road from micron-sized grains to fully grown planets is all but smooth. I will present recent studies on the formation of planetesimals -- the building blocks of planets -- in models of protoplanetary disks that account for turbulence, stratification, and magnetic fields, which have not been considered in this context. I will describe new difficulties, but also possible new paths to planet formation under these conditions.

[2]

### **TAO-DFT and Its Applications to Nanomaterials with Radical Nature**

Jeng-Da Chai<sup>1,2,3\*</sup>

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Abstract: I will briefly describe thermally-assisted-occupation density functional theory (TAO-DFT) [J.-D. Chai, J. Chem. Phys. 136, 154104 (2012)], density functional approximations in TAO-DFT (TAO-DFAs), hybrid TAO-DFT schemes (i.e., inclusion of exact exchange in TAO-DFT), self-consistent fictitious temperature scheme in TAO-DFT, and the applications of TAO-DFT to nanomaterials with radical nature (e.g., acenes, zigzag graphene nanoribbons, cyclacenes, Möbius cyclacenes, PAHs, linear carbon chains, linear boron chains, etc.). In contrast to Kohn-Sham density functional theory (KS-DFT), TAO-DFT is a density functional theory with fractional orbital occupations given by the Fermi-Dirac distribution (controlled by a fictitious temperature), for the study of large electronic systems with radical nature. Due to its computational efficiency and reasonable accuracy, TAO-DFT has been recently applied to the study of various nanomaterials with radical nature (i.e., challenging systems for conventional electronic structure methods). Some interesting results will be presented.

Keywords: TAO-DFT, static correlation, nanomaterials, radical nature, electronic properties.

[3]

**Supermetal-insulator transition in a non-Hermitian network model**

Jhih-Shih You

National Taiwan Normal University, Taipei, Taiwan

Abstract: We study a non-Hermitian and nonunitary version of the two-dimensional Chalker-Coddington network model with balanced gain and loss. This model belongs to the class  $D^{\text{dagger}}$  with particle-hole symmetry<sup>dagger</sup> and hosts both the non-Hermitian skin effect as well as exceptional points. By calculating its two-terminal transmission, we find a contact effect induced by the skin effect, which results in a nonquantized transmission for chiral edge states. In addition, the model exhibits an insulator to “supermetal” transition, across which the transmission changes from exponentially decaying with system size to exponentially growing with system size. In the clean system, the critical point separating insulator from supermetal is characterized by a non-Hermitian Dirac point that produces a quantized critical transmission of 4, instead of the value of 1 expected in Hermitian systems. This change in critical transmission is a consequence of the balanced gain and loss. When adding disorder to the system, we find a critical exponent for the divergence of the localization length  $\nu \approx 1$ , which is the same as that characterizing the universality class of two-dimensional Hermitian systems in class D. Our work provides a way of exploring the localization behavior of non-Hermitian systems, by using network models, which in the past proved versatile tools to describe Hermitian physics.

[4]

**An introduction to the NCTS-Physics**

Guang-Yu Guo

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Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan

Welcome to this NCTS Theoretical Physics Symposium in the 2022 TPS Annual Meeting. The National Center for Theoretical Sciences (NCTS) was established in August 1997 by the National Science Council (NSC) [NSC has become the Ministry of Science and Technology (MOST) since March 2014], and consists Mathematics and Physics Divisions. NCTS has entered its 5<sup>th</sup> phase since Jan. 2021. As the current Director of NCTS Physics Division, in the first 15 minutes of this talk, I will briefly introduce the present status of the Physics Division especially its organization structure, operation mode and major programs as well as its academic achievements in the past year. There will be 5 minutes for Q&A, and I will then try to response to the questions, comments, suggestions from the audience. More information can be found on the NCTS-Physics website <https://phys.ncts.ntu.edu.tw/>.

[5]

**The gravitational S-matrix**

Yu-tin Huang

Department of Physics, National Taiwan University, Taipei 10617, Taiwan

Recent revival of S-matrix bootstrap has been applied to a wide range of scenario, from constraining standard model effective field theory to constraining quantum gravity. In this talk I will present the state of the art constraints on low energy S-matrix of graviton amplitudes descending from a UV complete quantum gravity theory.

[6]

**Supernovae as astrophysical laboratories for fundamental physics**

Meng-Ru Wu

Institute of Physics, Academia Sinica, Taipei, Taiwan

Abstract: The core-collapse supernovae are among the most powerful explosions in the universe. The associated hot and dense conditions and the huge amount of released energy in different forms allow physicists to uniquely probe various fundamental physics issues beyond the reach of terrestrial laboratories. In this talk, I will discuss how different yet-unknown properties of neutrino physics and nuclear physics can affect the evolution of supernovae and the associated observables, and how we can use our understanding of supernovae to test different hypothetical particles beyond the Standard Model.

[7]

**Performance of quantum state transfer on IBM-Q, Ion-Q, and QuTech devices**

YI-TE HUAN<sup>1</sup>, JHENG-DONG LIN<sup>1</sup>, HUAN-YU KU<sup>1</sup>, YUEH-NAN CHEN<sup>1</sup>

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Quantum state transfer (QST) provides a method to send arbitrary quantum states from one system to another. Such a concept is crucial for transmitting quantum information into the quantum memory, quantum processor, and quantum network. In this talk, I will first introduce the concept of EPR steering. I will then describe the temporal analogue of EPR steering, i.e. temporal quantum steering. For practical applications, I will show that the temporal steerability is preserved when the perfect QST process is successful. Otherwise, it decreases under imperfect QST processes. We then apply the temporal steerability measurement technique to benchmark quantum devices including the IBM quantum experience, QuTech quantum inspire, and Ion-Q system under QST tasks. The experimental results show that the temporal steerability decreases as the circuit depth increases. Moreover, we show that the no-signaling in time condition could be violated because of the intrinsic non-Markovian effect of the devices

[8]

**Exciton-phonon dephasing and linewidth from first-principles in monolayer MoS<sub>2</sub>**

Y.-H. Chan<sup>1,2</sup>, Jonah B. Haber<sup>1</sup>, Mit H. Naik<sup>1</sup>, J. B. Neaton<sup>1</sup>, Diana Y. Qiu<sup>3</sup>, Felipe H. da Jornada<sup>4</sup>, and Steven G. Louie<sup>1</sup>

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Exciton-phonon interactions dominate the temperature dependence of the absorption and luminescence spectrum and determines exciton transfer rates on fs to ps time scales. However, the direct experimental measurement of exciton-phonon interaction is challenging and often subject to interpretation based on parameterized model Hamiltonians. We apply here a first-principles approach to study exciton-phonon coupling in monolayer MoS<sub>2</sub> and reveal the highly selective nature of exciton-phonon coupling due to the internal spin structure of excitons, which leads to a surprisingly long lifetimes of the lowest energy bright A exciton. Moreover, we show that interference terms due to off-diagonal exciton-phonon matrix elements, which have thus far been neglected in first-principles studies, are critical for the description of dephasing mechanisms, and once accounted for, yield exciton linewidths in excellent agreement with experiment.

This work was supported by the Center for Computational Study of Excited State Phenomena in Energy Materials (C2SEPEM), which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231. Y.H.C. acknowledges support by the Ministry of Science and Technology, National Center for Theoretical Sciences (Grant No. 110-2124-M-002-012 and 110-2112-M-001-018-MY3).