### The Chinese University of Hong Kong Division of Physics

### Theoretical Projects Offered in 2025-26

No.	Project title	Degree	Offered by
T1	Simulations of galaxies, dark matter, and the universe	MPhil or PhD	Prof. Tsang Keung Chan
T2	Turbulent double-diffusive convection	MPhil or PhD	Prof. Emily S. C. Ching
Т3	Topics in astrophysics and cosmology	MPhil or PhD	Prof. Ming Chung Chu
T4	Classification of topological phases of quantum matter in 3D		
Т5	Tensor network simulation in strongly correlated electron systems	PhD	Prof. Zhengcheng Gu
Т6	Using direct detections to study new gravitational-wave avenues	PhD or MPhil	Prof. Otto A. Hannuksela
Т7	Topological phases with higher symmetry in arbitrary dimensions	PhD	Prof. Tian Lan
Т8	Numerical studies of star formation	MPhil or PhD	<u>Prof. Hai-Bai Li</u>
Т9	Quantum physics, quantum sensing, and quantum foundation	PhD	Prof. Ren-Bao Liu
T10	Superradiant laser or maser		
T11	Searching for dark matter in astrophysical and cosmological observations	MPhil or PhD	Prof. Kenny C. Y. Ng
T12	Multi-messenger astrophysics and probes of fundamental physics		
T13	Computer modeling of Biomolecules	PhD or MPhil	Prof. Yi Wang
T14	Quantum simulation in theoretical cold-atom physics	PhD or MPhil	Prof. Yangqian Yan
T15	Few-body physics and thermodynamics of interacting Fermi gases		
T16	Doping and defects in semiconductor materials		
T17	Understanding long range magnetism in dilute magnetic semiconductors or topological materials	MPhil or PhD	Prof. Junyi Zhu

### T1. Simulations of galaxies, dark matter, and the universe (MPhil or PhD)

(Prof. T. K. Chan, tkchan@phy.cuhk.edu.hk)

Small inhomogeneities of the universe gravitationally collapse into dark matter halos. They are the birthplaces of stars and galaxies. Stars and galaxies inject energy and momentum back to gas, which suppresses new star formation. These galaxies also emit radiation and ionize the whole universe. We develop numerical methods and perform simulations to study cosmic structure formation, stellar feedback, and dark matter halos [1]. Our current focus is radiation feedback and cosmic reionization [2]. But we are also open to other relevant topics, including magnetohydrodynamics with cosmic rays [3] and application of machine learning in simulations.

#### References .

- 1. T. K. Chan et al., "The impact of baryonic physics on the structure of dark matter haloes: the view from the FIRE cosmological simulations", In: MNRAS 454.3, 2981-3001 (2015).
- 2. T. K. Chan et al., "Smoothed particle radiation hydrodynamics: two-moment method with local Eddington tensor closure", In: MNRAS 505.4, 5784-5814 (2021).
- 3. T. K. Chan et al., "Cosmic ray feedback in the FIRE simulations: constraining cosmic ray propagation with GeV y-ray emission", In: MNRAS 488.3, 3716-3744 (2019).

## **T2.** Turbulent double-diffusive convection (MPhil or PhD) (Prof. E. S. C. Ching, ■ ching@phy.cuhk.edu.hk)

In double-diffusive convection, fluid density depends on two components, temperature and its composition such as salt concentration, and fluid motion is driven by both temperature difference and compositional gradients. Turbulent double-diffusive convection plays an important role in oceanography and is crucial for ice-ocean interactions. Turbulent convection motion produced at the ice-ocean interface is driven by the temperature difference of ice and the ambient seawater as well as the salinity difference between the melt water and the surrounding salty seawater. The melting process of ice is controlled by a combination of heat and salinity transport. We will study turbulent double-diffusive convection in a vertical fluid layer and address the questions of how heat and salinity fluxes depend on parameters that control the flow. [Up to two students may be admitted.]

- 1. O. Shishkina, S. Horn, S. Wagner and E. S. C. Ching, "Thermal boundary layer equation for turbulent Rayleigh-Bénard convection", Phys. Rev. Lett. 114, 114302 (2015).
- E. S. C. Ching, H. S. Leung, L. Zwirner and O. Shishkina, "Velocity and thermal boundary layer equations for turbulent Rayleigh-Bénard convection", Phys. Rev. Research 1, 033037 (2019).
- 3. N. C. Tai, E. S. C. Ching, L. Zwirner and O. Shishkina, "Heat flux in turbulent Rayleigh-Bénard convection: Predictions derived from a boundary layer theory", Phys. Rev. Fluids 6, 033501 (2021).

4. E. S. C. Ching, "Heat flux and wall shear stress in large aspect-ratio turbulent vertical convection", Phys. Rev. Fluids 8, L022601 (2023).

### T3. Topics in astrophysics and cosmology (MPhil or PhD) (Prof. M. C. Chu, ■ mcchu@phy.cuhk.edu.hk)

Up to two students may be admitted to work on projects of mutual interest in theoretical astrophysics and cosmology, particularly on dark matter astrophysics and cosmology and neutrino cosmology. My current projects include Decaying Dark Matter Cosmology [1], Fuzzy Dark Matter Cosmology [2], Dark-matter Admixed Compact Stars [3], and Neutrino Cosmology [4].

#### References:

- 1. Jianxiong Chen and M.—C. Chu, "Metamorphosis of dwarf halo density profile under dark matter decays," to appear in The Astrophysical Journal, 2020; Dalong Cheng, M.-C. Chu and Jiayu Tang, "Cosmological Structure Formation in Decaying Dark Matter Models," Journal of Cosmology and Astroparticle Physics 07, 009 (2015).
- 2. Jiajun Zhang, Yue-Lin Sming Tsai, Jui-Lin Kuo, Kingman Cheung, and Ming-Chung Chu, "Ultralight Axion Dark Matter and Its Impact on Dark Halo Structure in N-body Simulations," The Astrophysical Journal 853, 51 (2018).
- 3. Shuai Zha, Ming-Chung Chu, Shing-Chi Leung, and Lap-Ming Lin, "Accretion-induced Collapse of Dark Matter Admixed White Dwarfs. II. Rotation and Gravitationalwave Signals," The Astrophysical Journal 883, 13 (2019); S.-C. Leung, M.-C. Chu, and L.-M. Lin, "Dark Matter Admixed Type IA Supernovae", Astrophysical Journal 812, 110 (2015).
- 4. Zhichao Zeng, Shek Yeung, Ming-Chung Chu, "Effects of neutrino mass and asymmetry on cosmological structure formation," Journal of Cosmology and Astroparticle Physics 03, 015 (2019).

### T4. Classification of topological phases of quantum matter in 3D (PhD)

(Prof. Z. C. Gu, **z**cgu@phy.cuhk.edu.hk)

The experimentally observed fractional quantum hall (FQH) states and topological insulators (TI) are examples of topological phases of quantum matter. How to systematically classify topological phases of quantum matter has become one of the most important open problems in modern condensed matter physics. In 2D, we have made a lot of progress along this direction based on the novel physical concept of long-range entanglement [1] and powerful mathematical framework of group cohomology theory [2,3]/tenser category theory [4]. One Ph D student may be admitted to work on the project of classifying topological phases of quantum matter in 3D. It is a joint project with Institute of Mathematics (IMS) at Chinese University of Hong Kong.

#### References:

- 1. Xie Chen, Zheng-Cheng Gu, Xiao-Gang Wen, Phys. Rev. B 82, 155138 (2010).
- 2. Xie Chen, Zheng-Cheng Gu, Zheng-Xin Liu and Xiao-Gang Wen, Science 338, 1604 (2012).
- 3. Zheng-Cheng Gu and Xiao-Gang Wen, Phys. Rev. B 90, 115141 (2014).
- 4. Alexei Kitaev, Annals of Physics, 321, 2 (2006).

### T5 Tensor network simulation in strongly correlated electron systems (PhD)

(Prof. Z. C. Gu, **z**cgu@phy.cuhk.edu.hk)

Due to strong electron correlation, the key mechanism of high temperature superconductivity remains to be one of the most challenge problems in modern condensed matter physics. In the past few years, we have developed very powerful tensor network algorithm[1,2,3,4] to simulate strongly correlated electron systems based on the novel concept of entanglement renormalization. One PhD student may be admitted to work on the project of developing tensor network algorithm to solve realistic strongly correlated systems, e.g., t-J/Hubbard model. For a long-term goal, we aim at developing an advanced "first principle" algorithm that can incorporate very strong electron correlations.

#### References:

- 1. Z. C. Gu, M. Levin and X.-G. Wen Phys. Rev. B 78, 205116 (2008).
- 2. Zheng-Cheng Gu and Xiao-Gang Wen Phys. Rev. B 80, 155131 (2009).
- 3. Zheng-Cheng Gu, Phys. Rev. B 88, 115139 (2013).
- 4. Shuo Yang, Zheng-Cheng Gu and Xiao-Gang Wen, arXiv:1512.04938 (2015).

#### T6. Using direct detections to study new gravitationalwave avenues (PhD or MPhil)

(Prof. O. A. Hannuksela,

in hannuksela@phy.cuhk.edu.hk)

Gravitational waves are the result of cataclysmic events that distort the fabric of space and time. The international LIGO collaboration made its first detection of the waves in 2015. Since then, two more detectors (Virgo in Italy and Kagra in Japan) have become operational. To name but a few discoveries enabled by the recent detections, they allowed us to gain access to the genuinely strong-field dynamics of spacetime, constrain the elusive neutron star equation of state, and arrive at an independent measurement of the Hubble constant [1]. More exciting scientific avenues are expected to become accessible in the future as we observe more gravitational waves at better sensitivities. We may admit one or more students to work on data-analysis projects. The focus topic will be gravitational-wave lensing [2-4], forecasted in the coming years. Still, broader topics, including inferring dark matter properties from gravitational waves [5-6], are also possible.

- 1. Miller, M. C., and Nicolás Y. "The new frontier of gravitational waves." Nature 568.7753 (2019): 469-476.
- 2. Hannuksela, O. A., et al. "Search for gravitational lensing signatures in LIGO-Virgo binary black hole events." The Astrophysical Journal Letters 874.1 (2019): L2.
- 3. Pang, P. T.H., et al. "Lensed or not lensed: determining lensing magnifications for binary neutron star mergers from a single detection." Monthly Notices of the Royal Astronomical Society 495.4 (2020): 3740-3750.
- 4. Hannuksela, O. A., et al. "Localizing merging black holes with sub-arcsecond precision using gravitational-wave lensing." Monthly Notices of the Royal Astronomical Society 498.3 (2020): 3395-3402.
- 5. Hannuksela, O. A., et al. "Probing the existence of ultralight bosons with a single gravitational-wave measurement." Nature Astronomy 3.5 (2019): 447-451.

6. Hannuksela, O. A., Ng, K. C. Y., and Li, T. G. F. "Extreme dark matter tests with extreme mass ratio inspirals." Physical Review D 102.10 (2020): 103022.

### T7. Topological phases with higher symmetry in arbitrary dimensions (PhD)

(Prof. T. Lan, tlan@cuhk.edu.hk)

Topological phases of quantum matter can have nontrivial and intriguing interplay with symmetry and higher symmetry. In two spatial dimensions, the symmetry enriched topological phases have been systematically understood using the concepts of G-crossed braided fusion category [1] and minimal modular extension [2,3,4].

Recently, combining the idea of boundary-bulk duality and categorical symmetry, a blueprint [5,6] has been proposed for higher dimensions. One PhD student may be admitted to study topological phases with higher symmetry in arbitrary dimensions. Strong mathematical background, especially in algebraic methods and category theory, is preferred.

#### References:

- 1. Barkeshli, M., Bonderson, P., Cheng, M. & Wang, Z., "Symmetry fractionalization, defects, and gauging of topological phases", Phys. Rev. B 100, 115147 (2019).
- 2. Lan, T., Kong, L. & Wen, X.-G., "Classification of (2+1)-dimensional topological order and symmetry-protected topological order for bosonic and fermionic systems with on-site symmetries", Phys. Rev. B 95, 235140 (2017).
- 3. Lan, T., Kong, L. & Wen, X.-G., "Modular extensions of unitary braided fusion categories and 2+1D topological/SPT orders with Symmetries", Commun. Math. Phys. 351, 709–739 (2017).
- 4. Lan, T., Kong, L. & Wen, X.-G., "Theory of (2+1)-dimensional fermionic topological orders and fermionic/bosonic topological orders with symmetries", Phys. Rev. B 94, 155113 (2016).
- Kong, L., Lan, T., Wen, X.-G., Zhang, Z.-H. & Zheng, H., "Classification of topological phases with finite internal symmetries in all dimensions", J. High Energy Phys. 2020, 93 (2020).
- 6. Kong, L., Lan, T., Wen, X.-G., Zhang, Z.-H. & Zheng, H., "Algebraic higher symmetry and categorical symmetry: A holographic and entanglement view of symmetry", Phys. Rev. Res. 2, 043086 (2020).

### **T8.** Numerical studies of star formation (MPhil or PhD) (Prof. H. B. Li, | hbli@cuhk.edu.hk)

Star formation is a complex process involving delicate interactions between, e.g. gravity, turbulence and magnetic fields (B-fields). Observations suggest that the shapes of molecular clouds (stellar nurseries), star formation rates and protester disk formation are all correlated with the orientation or strength of B-fields. We will use magnetohydrodynamic simulations to study how exactly these correlations can happen.

#### References :

- 1. "Self-similar Fragmentation Regulated by Magnetic Fields in a Region Forming Massive Stars", Nature 520, 518 (2015). [Link to Paper]
- 2. "Magnetic Fields in Molecular Clouds—Observation and Interpretation. [Link to Paper]
- 3. "The Link between Magnetic-field Orientations and Star Formation Rates". [Link to Paper]

4. "Turbulence in Zeeman Measurements from Molecular Clouds", Zhuo Cao (Ph.D. student) and Hua-bai Li, ApJL, 946, L46 (2023). [Link to Paper]

### T9. Quantum physics, quantum sensing, and quantum foundation (1 PhD)

(Prof. R. B. Liu, rbliu@cuhk.edu.hk)

One student is to be admitted to study in theory of quantum coherence control in solid-state systems, quantum sensing theory, and fundamental issues in quantum physics and statistical physics. The topics include (1) quantum many-body effects in mesoscopic spin baths, (2) quantum sensing using higher-order correlations of quantum objects and generalization of conventional nonlinear optics to quantum nolinear spectroscopy, (3) quantum dynamics of spin networks, and (4) dynamical phase transitions. Honesty, strong motivation, and hard working are must. Required is good training in quantum mechanics, solid-state physics, and computational physics at the undergraduate level.

#### References:

- 1. J. Meinel, et al, "Quantum nonlinear spectroscopy of single nuclear spins", Nature Communications 13, 5318 (2022)
- 2. P. Wang, et al, "Classical-Noise-Free Sensing Based on Quantum Correlation Measurement". Chinese Physics Letters 38, 010301 (2021)
- 3. P. Wang, et al., "Characterization of Arbitrary-Order Correlations in Quantum Baths by Weak Measurement", Physical Review Letters 123, 050603 (2019).
- 4. W. Yang, W. L. Ma and R. B. Liu, "Quantum many-body theory for electron spin decoherence in nanoscale nuclear spin baths", Reports on Progress in Physics 80, 016001 (2017).
- 5. B. B. Wei and R. B. Liu, "Lee-Yang zeros and critical times in decoherence of a probe spin coupled to a bath", Physical Review Letters 109, 185701 (2012).
- 6. N. Zhao, et al., "Atomic-scale magnetometry of distant nuclear spin clusters via nitrogen-vacancy spin in diamond", Nature Nanotechnology 6, 242 (2011).
- 7. J. Du, et tal., "Preserving electron spin coherence in solids by optimal dynamical decoupling", Nature 461, 1265-1268 (2009).

#### T10. Superradiant laser or maser (1 PhD)

(Prof. R. B. Liu, 🖃 rbliu@cuhk.edu.hk)

One student is to be admitted to study in theory superradiance and subradiance of quantum many-body systems and novel lasers and masers. Honesty, strong motivation, and hard working are must. Required is good training in quantum mechanics, solid-state physics, and computational physics at the undergraduate level.

- 1. R. B. Liu, "A masing ladder", Science 371, 780 (2021).
- 2. L. Jin, et al., "Proposal for a room-temperature diamond maser", Nature Communications 6, 8251 (2015).
- 3. D. W. Wang, et al., "Superradiance lattice", Physical Review Letters 114, 043602 (2015).

### T11. Searching for dark matter in astrophysical and cosmological observations (MPhil or PhD)

(Prof. K. C. Y. Ng, \subseteq kcyng@phy.cuhk.edu.hk)

Many astrophysical and cosmological observations have shown that much of the matter in the Universe is made of a substance that cannot be described by the Standard Model of particle physics. Identifying the nature of dark matter is one of the most important problems in modern science, and may provide clues to other important problems of Nature (neutrino mass, matter-antimatter asymmetry, etc). We will be looking into various astrophysical and cosmological probes to explore particle signatures of dark matter; examples of candidates are weakly interacting massive particles (wimps), axions, primordial black holes, etc. Depending on mutual interest, the projects may involve dark matter phenomenology in astro/cosmo setting [1,2], data analysis to search for dark matter [3], or exploring new ways (analysis techniques or physical observables) for more sensitive search [4]. These works will connect heavily with theoretical cosmology and high-energy astrophysics. One candidate may be considered. Please feel free to contact me directly for more information.

#### References:

- 1. Rebecca K. Leane, Tracy R. Slatyer, John F. Beacom, Kenny C. Y. Ng, "GeV-Scale Thermal WIMPs: Not Even Slightly Dead", Phys. Rev. D 98, 023016 (2018) [arXiv: 1805.10305].
- 2. Christopher V. Cappiello, Kenny C. Y. Ng, John F. Beacom, "Reverse Direct Detection: Cosmic Ray Scattering With Light Dark Matter", Phys. Rev. D99 (2019) no.6, 063004 [arXiv: 1810.07705].
- 3. Kerstin Perez, Kenny C. Y. Ng, John F. Beacom, Cora Hersh, Shunsaku Horiuchi, Roman Krivonos, "(Almost) Closing the Sterile Neutrino Dark Matter Window with NuSTAR", Phys. Rev. D 95, 123002 (2017) [arXiv: 1609.00667].
- 4. Eric G. Speckhard, Kenny C. Y. Ng, John F. Beacom, Ranjan Laha, "Dark Matter Velocity Spectroscopy", Phys .Rev. Lett. 116 (2016) no.3, 031301 [arXiv: 1507.04744].

# T12 Multi-messenger astrophysics and probes of fundamental physics (MPhil or PhD)

(Prof. K. C. Y. Ng, \subseteq kcyng@phy.cuhk.edu.hk)

In contrast to traditional astronomy, in which light is the main tool, Multi-messenger astrophysics adds the usage of cosmic rays, neutrinos, gravitational waves and more for understanding the Universe. These new messengers open the window to the most extreme environments in the Universe and are crucial for answering key problems such as the origin of cosmic rays, the mechanisms responsible for accelerating cosmic rays to ultra-high energy (> 10^22 eV), properties of the black holes, the fate of the Universe, etc. We will be exploring a wide range of currently open problems in astrophysics and cosmology, which may include observational and theoretical studies of how cosmic rays interact with the Sun, producing high energy gamma rays and neutrinos [1,2], as well as other topics [3]. When the opportunity arises, these works may also connect to tests of fundamental physics (dark matter, neutrino physics, etc [4]). One candidate may be considered. Please feel free to contact me directly for more information.

#### References:

- 1. Tim Linden, Bei Zhou, John F. Beacom, Annika H.G. Peter, Kenny C.Y. Ng, Qing-Wen Tang, "Evidence for a New Component of High-Energy Solar Gamma-Ray Production", Phys. Rev. Lett. 121, 131103 [arXiv: 1803.05436].
- 2. Bei Zhou, Kenny C. Y. Ng, John F. Beacom, Annika H. G. Peter, "TeV Solar Gamma Rays From Cosmic-Ray Interactions", Phys.Rev. D96 (2017) no.2, 023015 [arXiv: 1612.02420].
- 3. Kfir Blum, Kenny Chun Yu Ng, Ryosuke Sato, Masahiro Takimoto, 'Cosmic rays, anti-helium, and an old navy spotlight', Phys.Rev. D96 (2017) no.10, 103021 [arXiv: 1704.05431].
- 4. Otto A. Hannuksela, Kenny C. Y. Ng, Tjonnie G. F. Li, "Extreme Dark Matter Tests with Extreme Mass Ratio Inspirals", [arXiv: 1906.11845].

### T13. Computer modeling of Biomolecules (PhD or MPhil) (Prof. Y. Wang, www. yiwang. cuhk.edu.hk)

Our research is focused on using computational methods to understand the biological world at a molecular level. At this level, the basic components of life are four types of macromolecules: proteins, nucleic acids, lipids, carbohydrates. With the help of both supercomputers and gaming GPUs, we can model the motion of individual atoms of the above macromolecules and extract useful information about their structure, function and dynamics based on principles of statistical mechanics. Current work in our group revolves around lipid membranes and proteins, where we use modeling and simulations to understand, for example, how drug-like molecules get through a membrane [1], how an enzyme recognizes its substrates [2], as well as how a solution undergoes phase transition to form coacervate or hydrogel [3-4]. Computational approachs used in our group range from molecular dynamics simulations and free energy calculations to continuum modeling. Students with a keen interest in computer modeling of biomolecules are encouraged to apply, although no prior biology background is required. [1 to 2 PhD or MPhil students may be admitted.]

- 1. C-H Tse, et. al, "Affordable membrane permeability calculations: Permeation of short-chain alcohols through pure-lipid bilayers and a mammalian cell membrane". Journal of Chemical Theory and Computation 15, 2913-2924, 2019.
- 2. M. P. Torrens-Spence, et. al, "Structural basis for divergent and convergent evolution of catalytic machineries in plant aromatic amino acid decarboxylase proteins". Proceedings of the National Academy of Sciences 117(20), 10806-10817, 2020.
- 3. B. Yang, et. al, "Enhanced mechanosensing of cells in synthetic 3D matrix with controlled biophysical dynamics", Nature Communications 12, 3514, 2021.
- 4. X. Peng, et. al, "Coacervate-derived hydrogel with effective water repulsion and robust underwater bioadhesion promotes wound healing", Advanced Science 9, 2203890, 2022.

### T14 Quantum simulation in theoretical cold-atom physics (PhD or MPhil)

(Prof. Y. Q. Yan, yqyan@cuhk.edu.hk)

Ultracold atoms have been serving as a highly tunable platform that can simulate quantum systems from other fields including condensed matter, high energy, and astrophysics, etc. For example, one could simulate topological states of matter and SU(N) Fermi gases [1-3]. These works either are directly relevant to cold atom experiments or involve collaborations with experimentalists. First, we find the underlying physical picture behind the cold atom experiments in the literature. Then, we improve and propose new quantum simulation experiments.

Meanwhile we will learn to harness the power of modern computer. High level programming languages like Mathematica/Matlab, Python, etc. are expected to be used.

We will use various tools such as exact diagonalization, effective Hamiltonian, perturbation theory, mean-field approach (Gross-Pitaevskii equation), and tensor networks (density matrix renormalization group and time-evolution block-decimation), etc., to approximate and simulate what is happening in the experiments. We are interested in both equilibrium (ground state or finite temperature) and non-equilibrium dynamics (quench and periodically driven/Floquet dynamics). Relevant experimental platforms include harmonically trapped systems, quantum gases in optical lattices, 2D boxed systems, Rydberg atoms in a cavity, etc.

#### References:

- 1. Yangqian Ya, and Qi Zhou "Yang monopoles and emergent three-dimensional topological defects in interacting bosons", Phys. Rev. Lett. 120, 235302 (2018).
- 2. Yangqian Yan et. al. "Emergent periodic and quasiperiodic lattices on surfaces of synthetic hall tori and synthetic hall cylinders", Phys. Rev. Lett. 123, 260405 (2019).
- 3. Bo Song, Yangqian Yan, et. al., "Evidence for bosonization in a three-dimensional gas of SU(N) fermions", Phys. Rev. X 10, 041053 (2020).

### T15. Few-body physics and thermodynamics of interacting Fermi gases (PhD or MPhil)

(Prof. Y. Q. Yan, yqyan@cuhk.edu.hk)

Strongly interacting Fermi gases manifest themselves in nature in different forms, from neutrons in neutron stars to electrons in solids. Here, we are particularly interested in the dilute limit, where the range of interaction is much smaller than the interparticle spacing and interaction could be characterized by a single s-wave scattering length. The unitary Fermi gas emerges as the s-wave scattering length diverges. It is relevant to physical systems on different scales, e.g., cold atoms, nuclear physics, and astrophysics. We will learn and use various numerical methods such as variational Monte Carlo, finite temperature and ground state path integral Monte Carlo, diffusion Monte Carlo, machine learning, etc. to calculate the ground state and finite temperature properties of the unitary Fermi gas [1-4]. We will study few-body problems and use top-down and bottom-up approaches to connect them to the many-body system.

We are also interested in slightly different systems and the aforementioned numerical tools could be applied to them as well. For example, we would study weakly interacting p-wave Fermi gas, which should be much simpler, strongly interacting Bose droplet, which brings Efimov physics [5] to the table, etc.

We expect to develop parallel computing code using suitable computer languages, e.g., CUDA, C++ with OpenMP/MPI, Python, Mathematica. Linux, version control, and many other modern computer tools will be used, which I believe will be useful no matter which path you take as you venture into the future.

#### References:

- 1. Yangqian Yan and D. Blume, "Path-integral Monte Carlo determination of the fourth-order virial coefficient for a unitary two-component Fermi gas with zero-range interactions", Phys. Rev. Lett. 116, 230401 (2016).
- 2. Yangqian Yan and D. Blume, "Abnormal superfluid fraction of harmonically trapped few-Fermion systems", Phys. Rev. Lett. 112, 235301 (2014).
- 3. Yangqian Yan and D. Blume, "Energy and structural properties of N-boson clusters attached to three-body Efimov states: Two-body zero-range interactions and the role of the three-body regulator", Phys. Rev. A 92, 033626 (2015).
- 4. Yangqian Yan and D. Blume "Harmonically trapped Fermi gas: Temperature dependence of the Tan contact", Phys. Rev. A 88, 023616 (2013).
- 5. D. Blume and Yangqian Yan, "Generalized Efimov scenario for heavy-light mixtures", Phys. Rev. Lett. 113, 213201 (2014).

### T16. Doping and defects in semiconductor materials (MPhil or PhD)

(Prof. J. Y. Zhu, i jyzhu@phy.cuhk.edu.hk)

Doping is one of the most important topics in semiconductor materials. A very small amount of foreign element may greatly change the electronic and optical properties of semiconductor materials. Tuning dopants and defects can be a promising strategy to greatly improve device performance. To understand doping mechanisms, investigate electronic structures, and simulate thermal and kinetic processes of doping, density functional theory (DFT) calculations have been proved to be effective tools. Accurate DFT calculations are the state of art techniques in solving important material physics problems. Our goals are: investigation of defects and doping of semiconductors and their alloys (InGaN, AlGaP, CZTS, CIGS, SiC, diamond), which are very important solid state lighting, photo voltaic, and information materials. Defects and dopant formation energies and transition energies will be calculated. New strategies of tuning defects and dopants will be proposed. With close collaborations with experimental groups, we expect our findings will greatly enhance the performance of the semiconductor materials. [One student may be admitted.]

- 1. T. Kuykendall, P. Ulrich, S. Aloni and Peidong Yang, "Complete composition tunability of InGaN nanowires using a combinatorial approach", Nature Materials 6, 951 956 (2007).
- 2. A. Walsh, S. Y. Chen, S. H. Wei and X. G. Gong, "Kesterite thin-film solar cells: advances in materials modelling of Cu<sub>2</sub>ZnSnS<sub>4</sub>", Advanced Energy Materials 24, 2305-2309 (2012).
- 3. J. Y. Zhu, F. Liu and G. B. Stringfellow, S. H. Wei, "Strain-enhanced doping in semiconductors: effects of dopant size and charge state", Phys. Rev. Lett. 105, 195503 (2010).

# T17. Understanding long range magnetism in dilute magnetic semiconductors or topological materials (MPhil or PhD)

(Prof. J. Y. Zhu, 🖃 jyzhu@phy.cuhk.edu.hk)

Magnetic semiconductors have attracted vast research interests because of the new physics and great potential in devices and applications. The recent discoveries of quantum anomalous Hall effect demonstrates the importance of long range magnetism in carrier free materials. However, there lack fundamental understandings of long range magnetic order in such semiconductors or topological materials. To understand the long range magnetic coupling in various compounds, we'll apply density functional theory studies to investigate the structure, electronic, and magnetic properties of various dilute magnetic semiconductors or topological materials. Our goals are: searching of new materials with strong magnetic coupling strength and stable magnetic phases, understanding how band topology affects the magnetic coupling, discoveries of the new microscopic origin of the magnetic phases, design of new magnetic devices based on the new mechanisms. [One student may be admitted.]

- C. Z. Chang, J. Zhang, X. Feng, J. Shen, Z. Zhang, M. Guo, K. Li, Y. Ou, P. Wei, L. L. Wang, et al., Science 340, 167 (2013).
- 2. B. Deng, Y. O. Zhang, S. B. Zhang, Y. Y. Wang, K. He, and J. Y. Zhu, Phys. Rev. B 94, 054113 (2016).
- 3. C. K. Chan, X. D. Zhang, Y. O. Zhang, K. F. Tse, B. Deng, J. Z. Zhang and J. Y. Zhu, "Step Stone Effect: A sp antibonding Mediated Long-Range Ferromagnetism in Crdoped Carrier-Free Bi2Te3", arXiv:1701.04943. (2017)