A3 group (Condensed-matter theory)

Graduate course

(A3 group is the sub-group at the entrance exam. of grad. course.)

Department of Physics (Hongo)	6 faculty members
Institute for Solid State Physics (Kashiwa)	6 faculty members
Department of Basic Science (Komaba)	2 faculty members
Institute of Industrial Science (Komaba2)	1 faculty members

Graduate students

Department of Physics (Hongo) 6 faculty members

Master course	22	(11/year)
Doctor course PhD	29	(9.7/year)

S. Miyashita Retired in 2019 (Statistical mechanics, nonequilibrium)

Now we are advertising a new faculty position (for rather young faculty member)

A3 group (Condensed-matter theory)

Masao Ogata	Strongly correlated electron systems, High-Tc, Dirac electrons, Topological materials, Thermoelectric properties
Shinji Tsuneyuki	Development of methods in first-principles calculations, Thermal conductivity, Dielectric properties, High pressure, Surfaces
Masahito Ueda	Cold atom systems, Nonequilibrium, Information thermodynamics, Machine learning
Mio Murao	Quantum information, Foundation of quantum mechanics
Synge Todo	Development of Monte Carlo methods, Spin systems, Phase transition, Critical phenomena, Machine learning
Hosho Katsura	Strongly correlated systems, Topological materials, Exactly solvable models

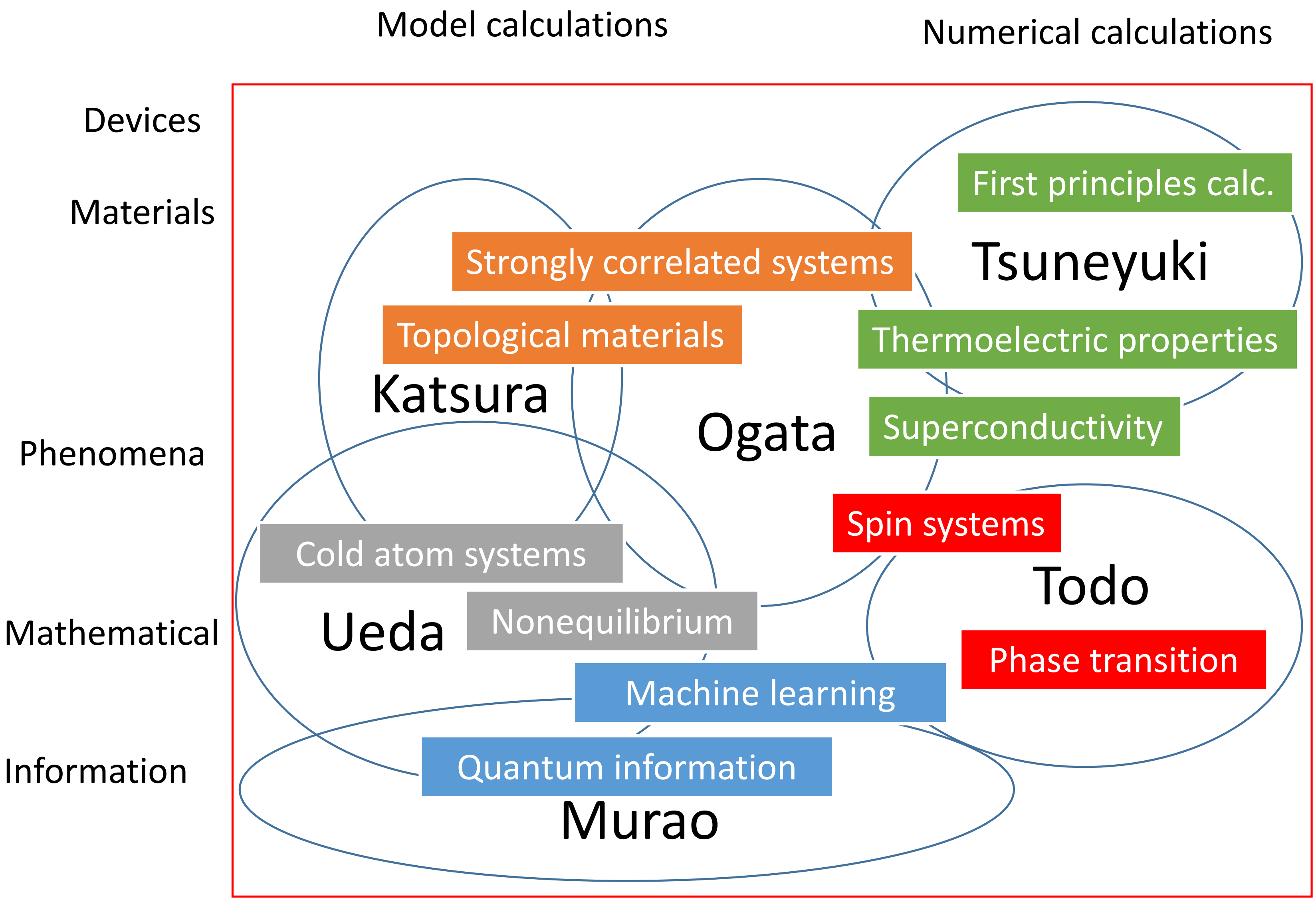
A3 group (Condensed-matter theory)

A few decades ago

Solid state physics
Semiconductor (Y. Uemura, H. Kamimura)
  Surface sciences, First-principles calculations
  High magnetic field, Quantum Hall effect
  Superconductivity
Statistical Mechanics (R. Kubo, M. Suzuki)
  Critical Phenomena
  Renormalization group, Kondo effect
  Exactly solvable models

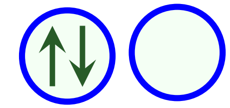
Plasma physics
Fluid dynamics

A3 group (Condensed-matter theory)



Ogata group 1: Mott metal-ins. transition and supercond.

Variational wave function (Hubbard model)



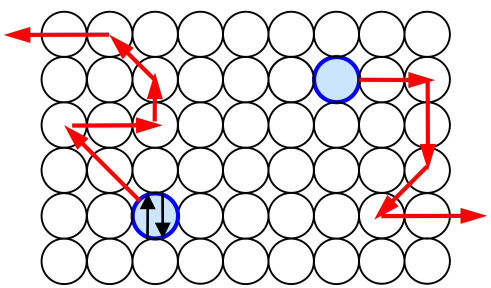
$$\Psi_{SC} = \mathcal{P}_Q \mathcal{P}_G |\mathrm{BCS}(\Delta)\rangle$$

RVB insulator

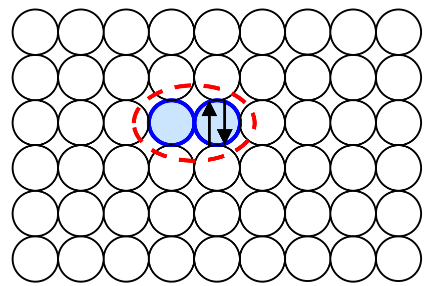
new projection operator controlling
the correlation between doublons and holons is **Essential**

- $\delta = 0$

free doublon & holon ↔ **bound state**

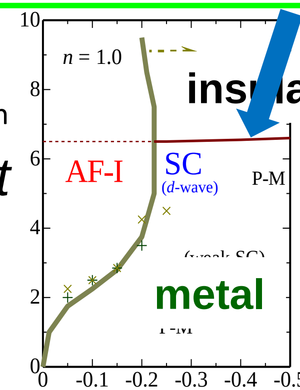


metal

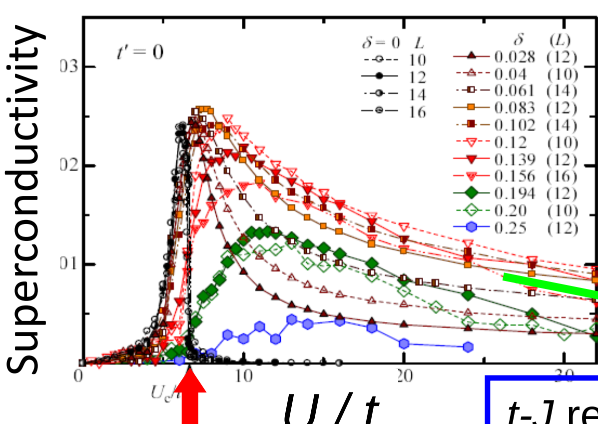


insulator

Mott transition as a first-order phase transition (like gas-liquid)



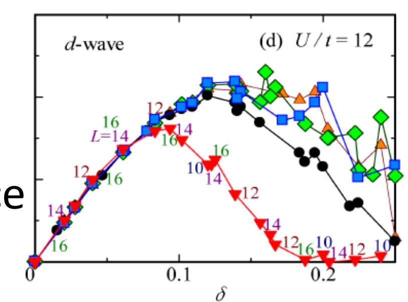
- $\delta \neq 0$



Superconductivity:
Crossover from weak to strong = Doped Mott ins.

t-J region

Doping dependence



Ogata group 2: Dirac electrons, Weyl semimetal

- Bismuth (3-dim. Dirac electrons)

Large orbital (dia) susceptibility in insulating $Bi_{1-x}Sb_x$ — χ_m

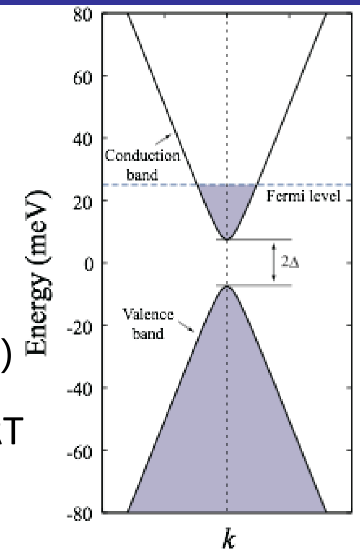
Large permittivity (dielectric constant) — ε

Large spin Hall coefficient (theoretical prediction) — σ_{SHE}

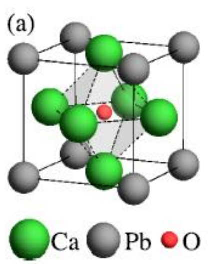
$$e\sigma^i_{sjk} = \begin{cases} 8,000-1,600 & (xy\ \text{plane}) \\ 18,000-36,000 & (yz\ \text{plane}) \\ 18,000-36,000 & (zx\ \text{plane}) \end{cases} \quad \Omega^{-1}\mathrm{cm}^{-1}$$

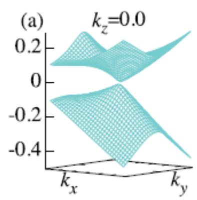
due to spin-orbit (SOC)

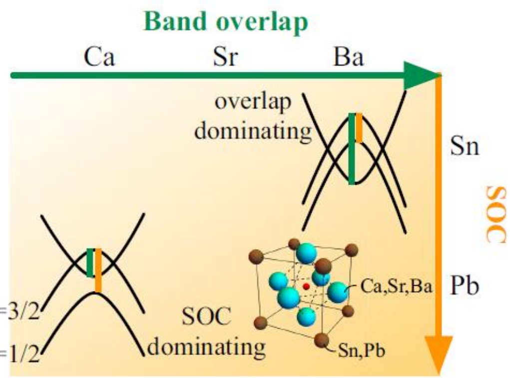
cf.) Pt: 240 $\Omega^{-1}\mathrm{cm}^{-1}$ @ RT

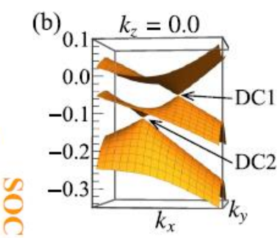


- Antiperovskite Ca_3PbO









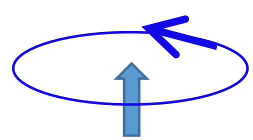
Twin Dirac

Kariyado Ogata
P. R. Materials **1**,
061201(R) (2017)

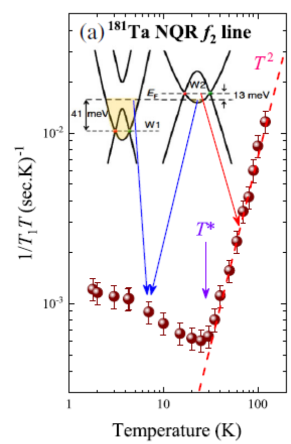
Experiments in Takagi group

- NMR $1/T_1$ due to orbital motion

$$\boldsymbol{a}_q = -i\mu_0\gamma_n \boldsymbol{I} \times \frac{\boldsymbol{q}}{|\boldsymbol{q}|^2}$$



$$\frac{1}{T_1} = \frac{e^2\mu_0^2\gamma_n^2}{18\pi c^2}(k_B T)^3 \ln\left(\frac{2k_B T}{\hbar\omega_n}\right)$$



Yasuoka et al PRL **118**, 236403 (2017) TaP

Maebashi et al.
J. Phys. Chem. Solids
128, 138 (2019)

- Orbital-Zeeman cross susceptibility

$$\chi_{\mathrm{OZ}} = \frac{2e\mu_B}{\hbar}\sum_{l:\mathrm{occ}}\sum_{\boldsymbol{k}}(\Omega^z_{l\uparrow} - \Omega^z_{l\uparrow}) = \frac{4e\mu_B L^2}{h}\sum_{l:\mathrm{occ}} \mathrm{Ch}_{s,l}$$

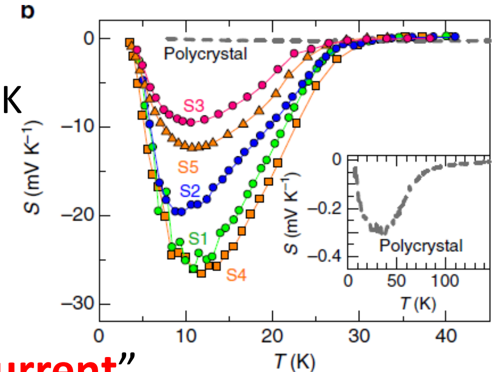
Ozaki and Ogata, in preparation

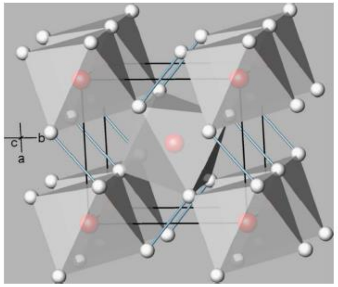
Ogata group 3: Thermoelectric properties

- Large Seebeck effects in $FeSb_2$

  more than 10 mV/K at 10K

  Probably due to **Phonon Drag**
  In disordered semiconductor





- Theoretical difficulty is in "**Heat current**"

  There are many kinds of heat currents !

  Thermal current carried by phonon

$$J_Q = J_Q^{\rm kin} + J_Q^{\rm imp} + J_Q^{\rm el-ph(1)} + J_Q^{\rm el-ph(2)} + J_Q^{\rm el-el(1)} + J_Q^{\rm el-el(2)} + J_Q^{\rm ph},$$

Ogata and Fukuyama,
J. Phys. Soc. Japan
88, 075703 (2019)

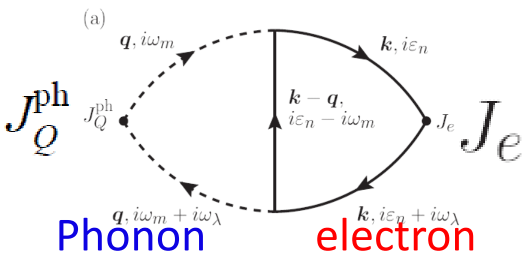
Part of J_Q gives the Mott formula.

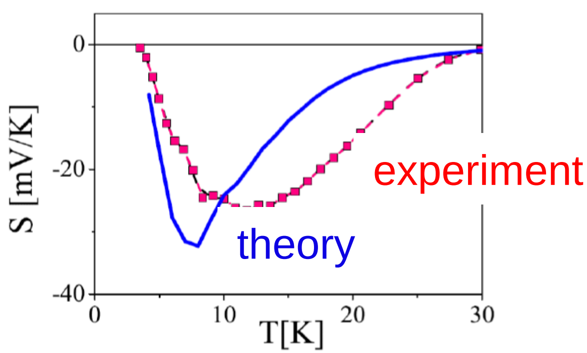
$$S = \frac{\pi^2}{3}\frac{k_B^2 T}{e}\left(\frac{d\ln\sigma(\varepsilon,0)}{d\varepsilon}\right)_{\varepsilon=\mu}$$

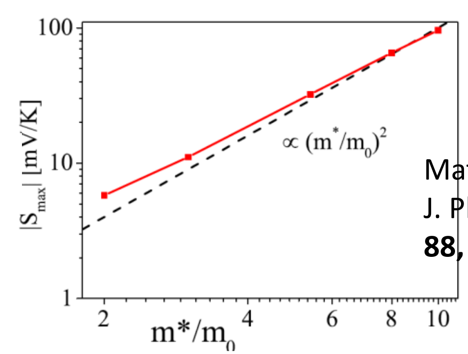
Same as in
Boltzmann eq.

Phonon drag mechanism is nothing to do with conductivity, i.e, not Mott formula.

- Application to $FeSb_2$





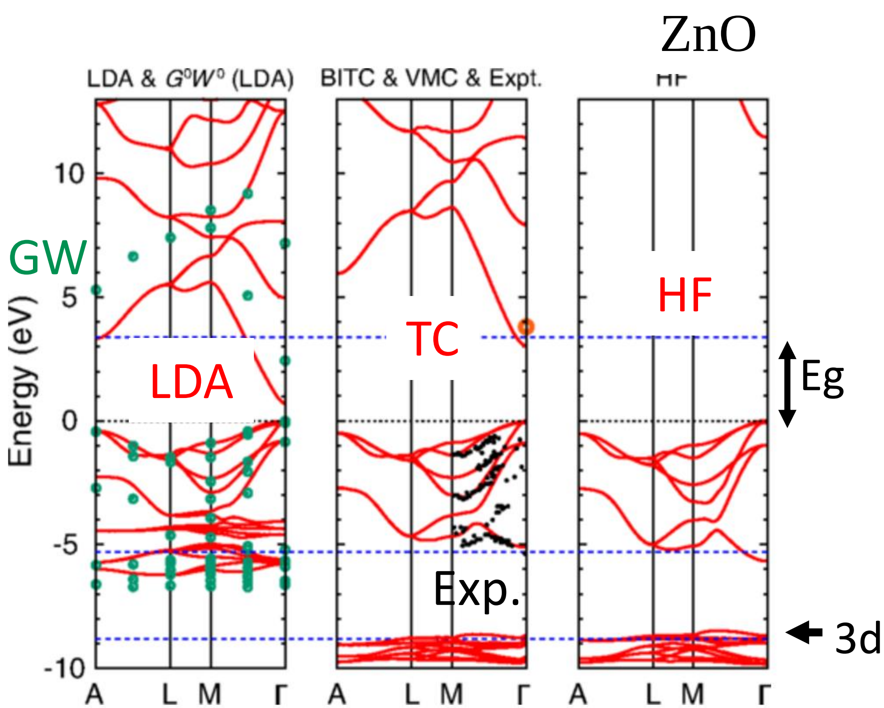


Matsuura et al,
J. Phys. Soc. Japan
88, 075601 (2019)

Tsuneyuki Group

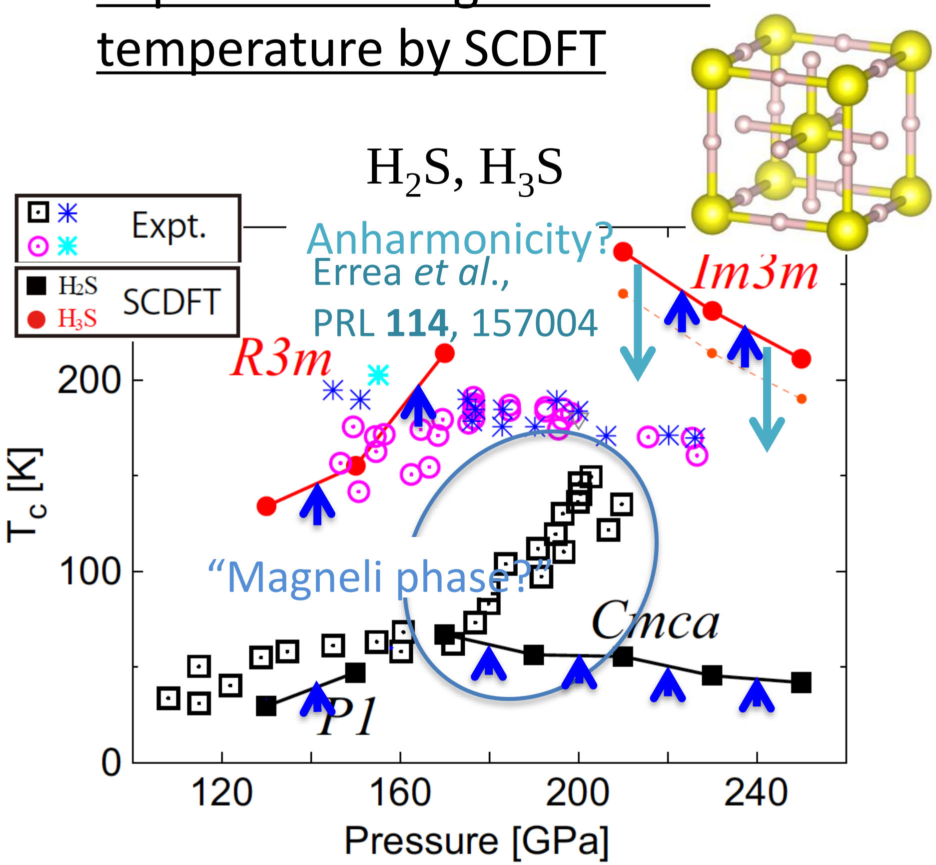
Development and applications of first-principles computer simulation methods for materials science

- Transcorrelated (TC) method: a wave function theory for condensed matter



M. Ochi, et al., Phys. Rev. Lett. 118, 026402 (2017).

- Superconducting transition temperature by SCDFT

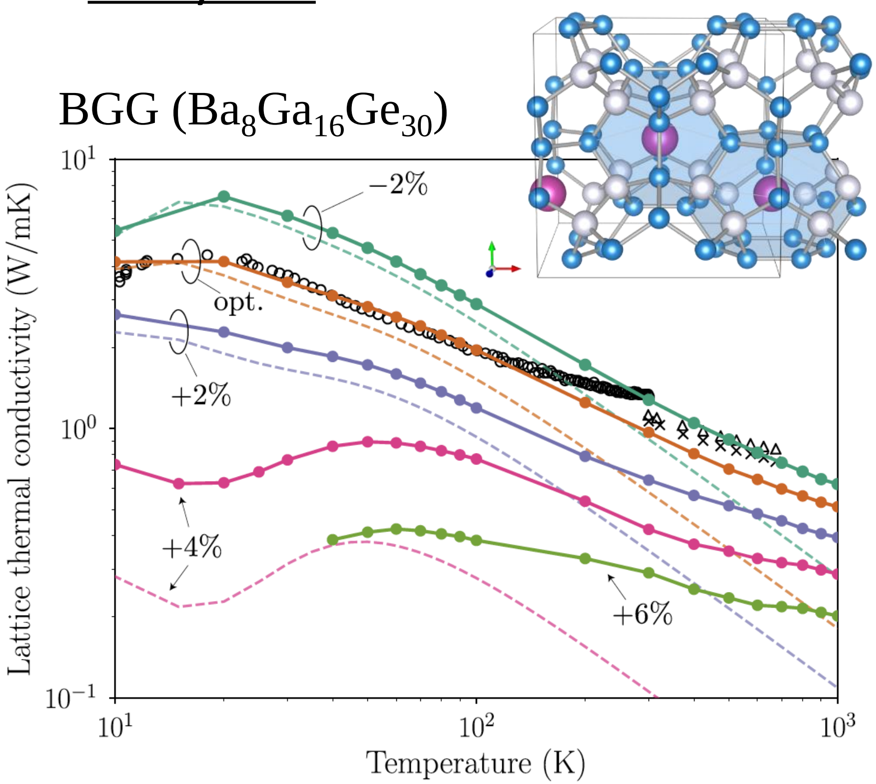


R. Akashi et al., Phys. Rev. B 91, 224513 (2015)

Tsuneyuki Group

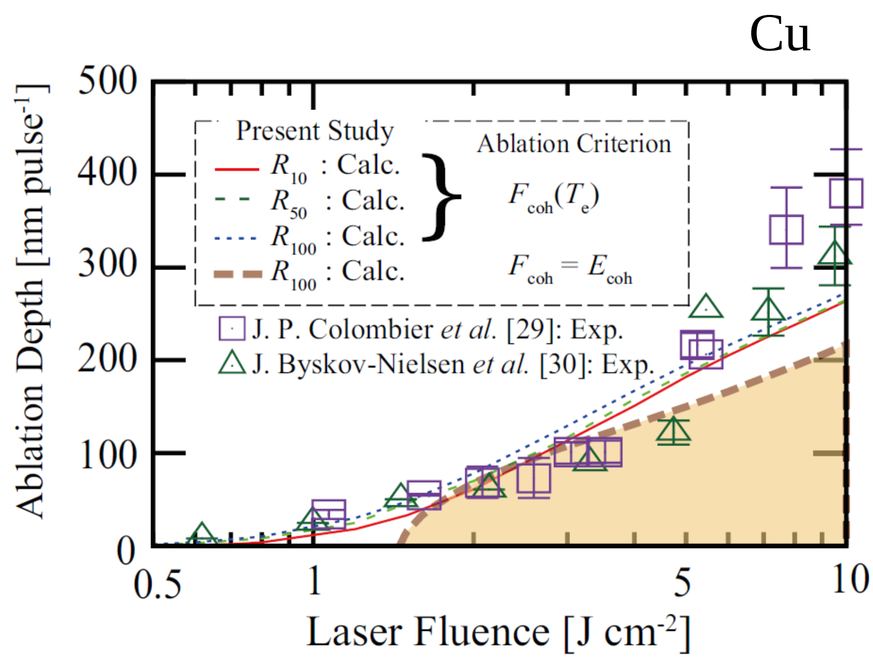
Development and applications of first-principles computer simulation methods for materials science

- Anharmonic phonon properties of crystals



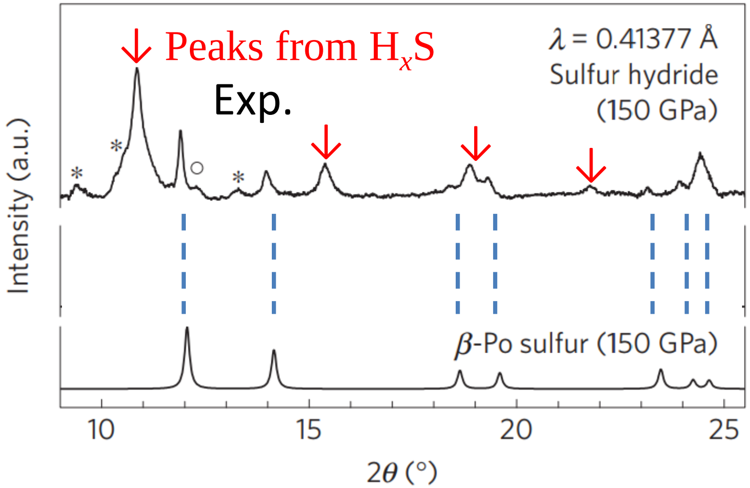
T. Tadano et al., Phys. Rev. Lett., 120, 105901 (2018).

- Non-thermal laser ablation of metals caused by electronic entropy



Y. Tanaka et al., Appl. Phys. Express 11, 046701 (2018)

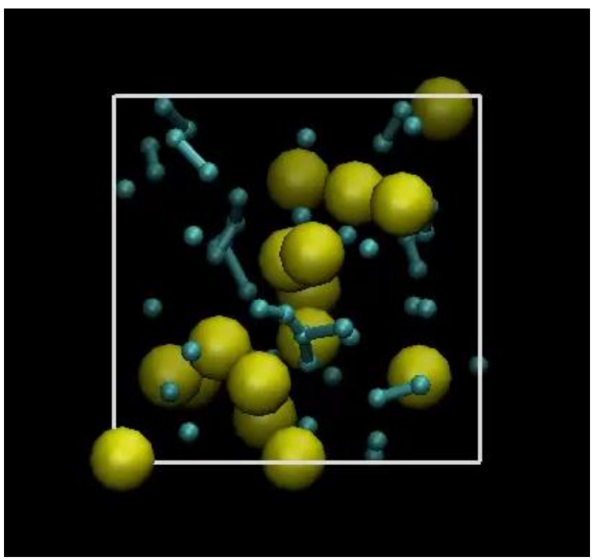
Tsuneyuki Group



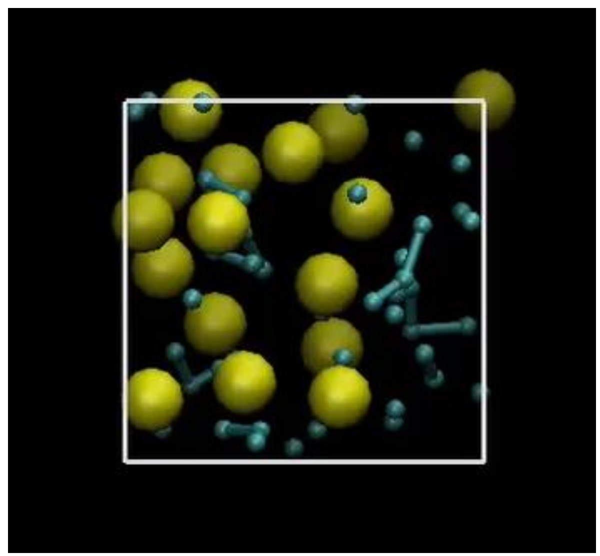
- <u>Data assimilation method for crystal structure prediction</u>

Position of hydrogen atoms cannot be determined by X-ray diffraction

Exp. Diffraction data are taken from M. Einaga et al., Nature Phys. (2016)



Simulated Annealing



Data Assimilation

We can obtain crystal structure by assimilating X-ray powder diffraction data much more easily compared with ordinary simulated annealing.

N. Tsujimoto et al., Phys. Rev. Materials 2, 053801 (2018).

Masahito Ueda (since 2008)

Research

- **Information thermodynamics** The paradox of Maxwell's demon had remained unresolved for more than one and half century, mainly because the quantitative analysis of the energy cost of measurement was difficult. By combining the Jarzynski equality with quantum theory of measurement , we have shown that the sum of the energy cost of measurement and that of the erasure always exceeds the free-energy gain by the demon. This work has developed into the field known as information thermodynamics.

- **Topological excitations in Bose-Einstein condensates** Ultracold atomic systems have unprecedented controllability to manipulate quantum gases. We have predicted a number of topological excitations such as chiral spin vortices, non-Abelian vortices and knots. Many of our predictions have been demonstrated experimentally.

- **Complete classification of non-Hermitian phases** Non-Hermitian physics has seen a remarkable development in situations with gain and loss or with postselection. We have made a complete classification of non-Hermitian topolocial phases with a total of 38 classes, in contrast to the Hermitian 10-fold Altrand-Zirnbauer classification. Such a complete classification will serve as a starting point to investigate topological phenomena in open quantum systems.

Research Plans

- Continue efforts to explore fundamental and foundational aspects of (low-energy) physics. In particular, I wish to study open quantum many-body phenomena and develop methods to do so.

- Extend the frontiers of physics and artificial intelligence by integrating them. I wish to understand why deep learning works so well in many different areas of optimization and classification problems. I am also interested in constructing explainable AI, that is, the AI that can explain the origin of the outcome.

Society services

2003-2009 Divisional Associate Editor of Physical Review Letters
2015-2016 Member of Central Council of Education (中教審教育企画特別部会)
2017-2018 Department deputy chief (2017) and chief (2018)
2016-present Editorial board member of Annual Review of Condensed Matter Physics
2018-present Editorial board member of Physical Review X
2018-present Research supervisor (研究総括) of CREST, JST

Education (since 2008)

Mentoring: 2 assistant profs.
→ 1 associate prof. (Nagoya), 1 lecturer (Keio)
14 postdocs → 8 assistant prof., 1 associate prof., 2 full prof.,
2 permanent research scientist (RIKEN, Hitach)
Supervised: 16 PhD students
→ 8 assis. prof., 2 assoc. prof., 1 permanent research scientist (NEC)
Currently 6 PhD students, 1 posdoc

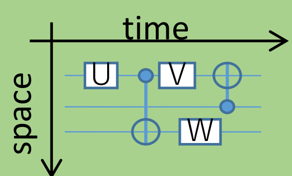
Murao Group: Theoretical Quantum Information

Our aim

By **using and programming quantum computers** that can implement any operations allowed by quantum mechanics, we answer the following questions of quantum nature:

How *does quantum mechanics power up information processing?*

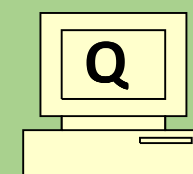
Better understanding of quantum physics under manipulation



basic science

very closely related!

applied science



What *can be done with quantum computers?*

Quantum algorithms and programming for quantum computers

In particular, we mainly focus on **quantum tasks/algorithms** and **distributed quantum information processing**

Inventing new quantum tasks/algorithms

toward a new paradigm of functional quantum programming

- *Focus on quantum algorithms for tasks with* ***quantum inputs and quantum (or classical) outputs*** *that cannot be handled by classical computers*
- *Aiming for developing a new framework of* ***functional quantum programming****, implementation algorithms of* ***higher-order quantum operations*** *are analyzed*
- *Analyze* ***causal order structures*** *in higher order quantum operations*
- *Seeking applications for quantum simulation, sensors and process controllers/processors*

<u>*Usual quantum computers*</u>
= quantum state processor

<u>*Higher-order quantum operations*</u>
= **quantum process processor**

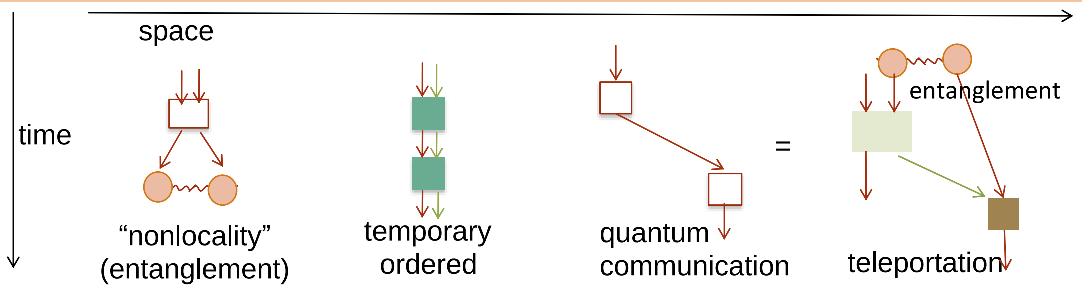
<u>Selected works</u>

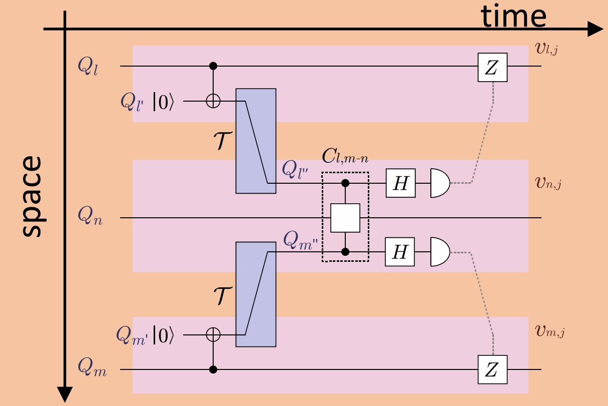
- Quantum algorithm for **projective measurement of energy** of **unknown** Hamiltonian systems, Nakayama, Soeda and Murao, Phys. Rev. Lett. (2015)
- Quantum algorithm for **inverting, transposing and conjugating unknown** unitary gates, Quintino, Dong, Shimbo, Soeda and Murao, Phys. Rev. Lett (2019)
- Quantum algorithm for **neutralizing and controlling** divisible **unknown** unitary gates, Dong, Nakayama, Soeda and Murao, submitted to PRX, arXiv:1911.01645 (2019)

Distributed quantum information processing

analysis of the spacetime structure in quantum computation

- *Distributed quantum information processing is a* ***network of small quantum computers distributed in space and time****, some quantum computation requires longer sequences (****complexity of causal structure****), some requires more entanglement (****nonlocal resources****)*





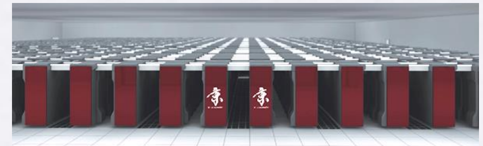
- *We analyze* ***causal structures****,* ***nonlocality*** *and* ***pararellizability*** *in quantum programming for achieving efficient distributed quantum information processing*

Selected works

- Formulation and analysis of **network coding for quantum computation** over butterfly and cluster networks, Akibue and Murao, IEEE Trans. Inf. Theory (2016)
- Analysis of **quantum communication cost** of distributed quantum information encoding and decoding, Yamasaki and Murao, IEEE Trans. Inf. Theory (2019)
- Analysis of the **tradeoff** between nonlocal resources and complexity of the causal structure in quantum programming, Wakakuwa, Soeda and Murao, Phys. Rev. Lett. (2019)

藤堂研究室 TODOGROUP

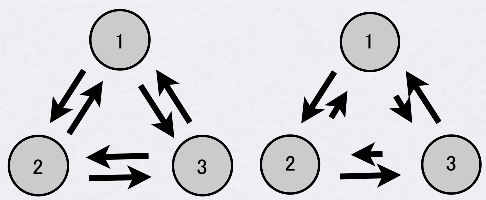
東京大学 THE UNIVERSITY OF TOKYO 大学院理学系研究科物理学専攻 / 物性研究所 DEPARTMENT OF PHYSICS / INSTITUTE FOR SOLID STATE PHYSICS



Computational Exploration of Quantum Many-body Phenomena

- Staff: Synge Todo (Professor), Tsuyoshi Okubo (Project Lecturer), Hidemaro Suwa (Assistant Professor)
- Research Highlight
  - Development of simulation algorithms for strongly-correlated many-body systems

Monte Carlo without detailed balance



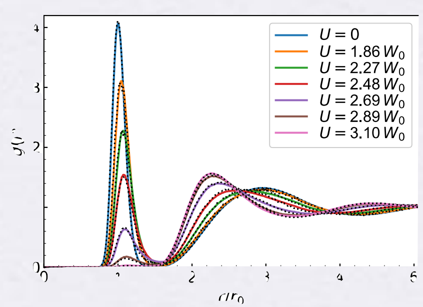
Tensor network algorithms

Quantum MC method for topological order

Order-N MC method for long-range interacting systems

  - Application of machine learning (ML) technique to materials science

ML force-field for molecular dynamics



Crystal structure prediction by data assimilation

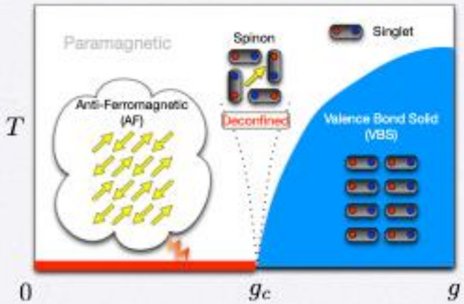
Materials informatics: search for rigid materials by ML

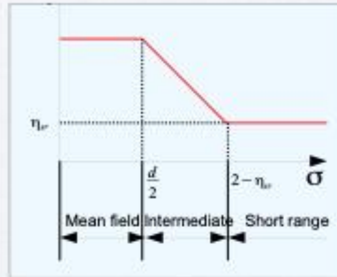
Detection of hidden order parameter by neural network

- Novel state and critical phenomena in strongly correlated systems

Deconfined critical phenomena

Spin system with long-range interaction





Field-induced magnetic order

Strongly anisotropic system

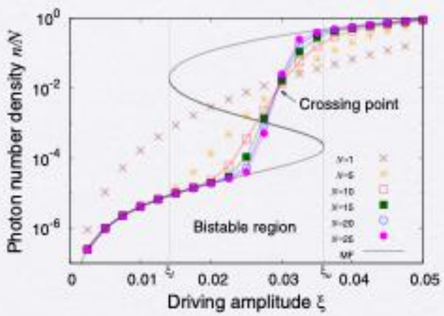
Supersolid in extended Hubbard model

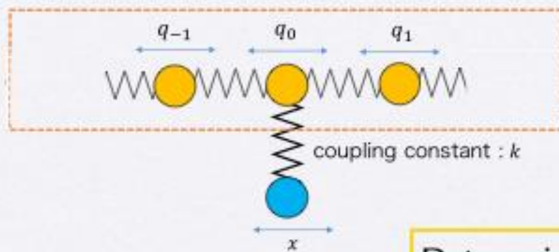
impurity induced long-range order

- Cooperative phenomena in non-equilibrium and non-steady states

Optical bistability in cavity system

Non-ergodicity in harmonic oscillators





Hybrid Algorithms for NISQ devises

Data assimilation for quantum device

- Development of open-source software for next-generation parallel simulations

Quantum lattice model solvers

MateriApps

TeNeS - Tensor network algorithm

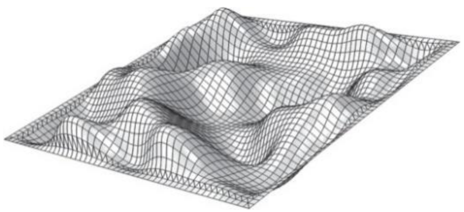
Quantum circuit simulator

ALPS

MateriApps LIVE!

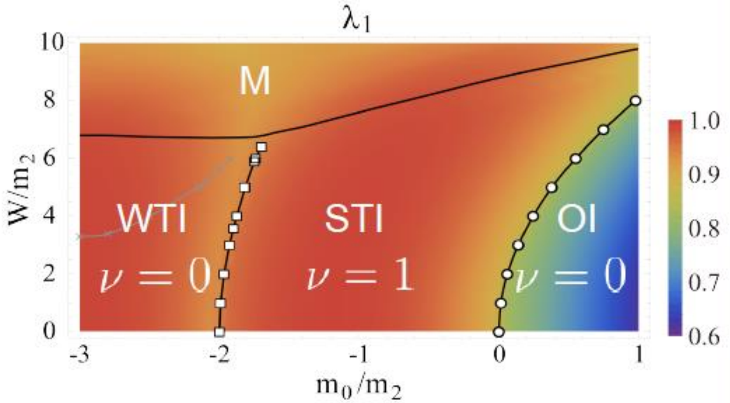
Katsura group: cond-mat theory & stat-mech

■ Disordered topological insulators (TIs)

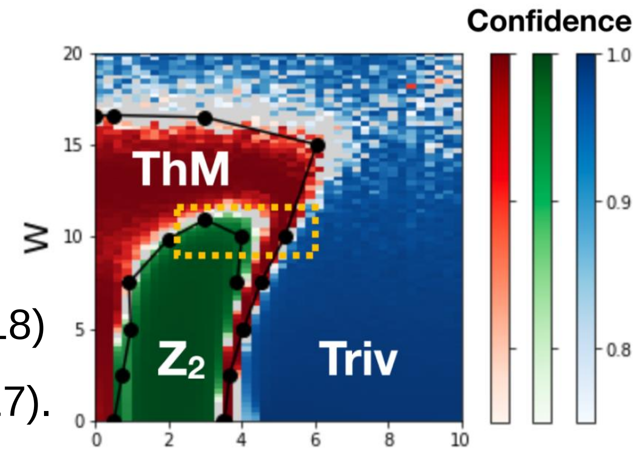


- TI: band insulators characterized by topological invariants e.g. Chern number
- How to characterize TI with disorder? NOTE) momentum is not conserved
- **Non-commutative geometry** approach
  Ex.) Z2 index for 3D TI in class AII

$$\nu = \dim\ker(P - DPD - 1) \mod 2$$



- **Machine learning** approach
  Feed wave functions to neural network
  Ex.) 2D class DIII topological SC



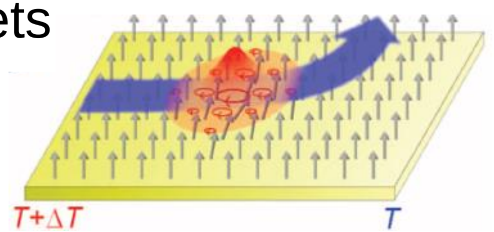
◆ Katsura and Koma, *J. Math. Phys*. **57** (2016); **59** (2018)

◆ Akagi, Katsura and Koma, *J. Phys. Soc. Jpn.* **86** (2017).

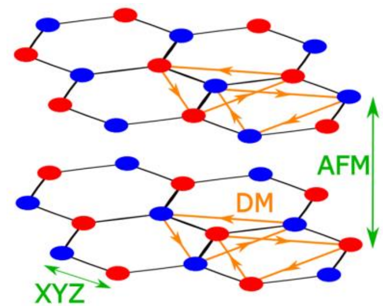
◆ Yoshioka, Akagi, and Katsura, *Phys. Rev. B* **97** (2018).

■ Topological magnon systems

- Magnon:
  elementary (bosonic) excitation in ordered magnets

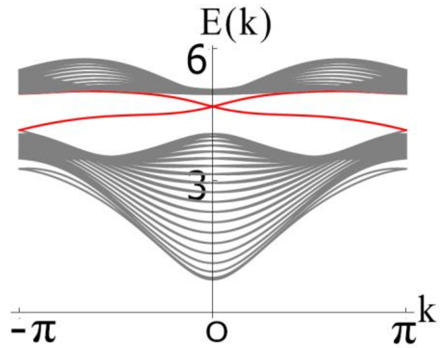


- Thermal Hall effect of magnons:
  Magnetic analog of integer quantum Hall effect
  Katsura *et al*., *Phys. Rev. Lett*. 104, 066403 (2010).



- What is a magnetic/bosonic analog of TI
  with time-reversal symmetry?

Up/down electrons ⟺ Bosons at ●/●



- Identified bosonic **Z2 topological invariant**
  Robust edge states, 3D generalizations

- Possible application to van der Waals magnets?
  Ex.) CrI_3 (bilayer, stack, …)

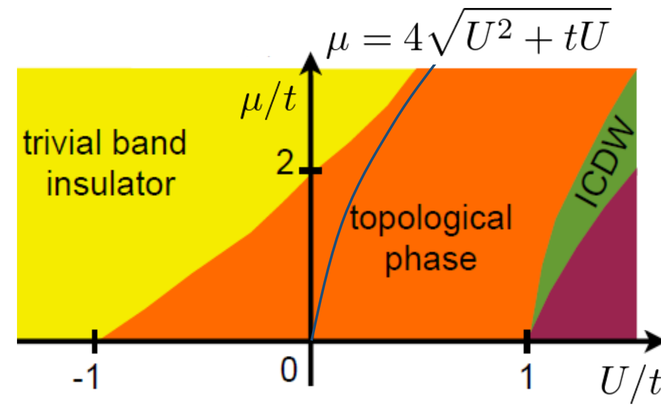
◆ 2D systems: Kondo, Akagi and Katsura, *Phys. Rev. B* **99** (2019).

◆ 3D systems: Kondo, Akagi and Katsura, *Phys. Rev. B* **100** (2019).

■ Interacting Majorana fermions

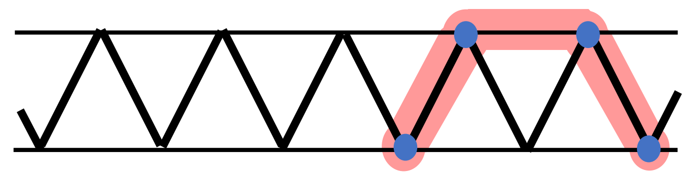
- Defining relations

$$(\gamma_i)^\dagger = \gamma_i, \quad \{\gamma_i, \gamma_j\} = 2\delta_{ij}$$



- Interacting Kitaev chain
  Exact ground states, topological order

- N=1 supersymmetric model
  NG fermion with **cubic dispersion**

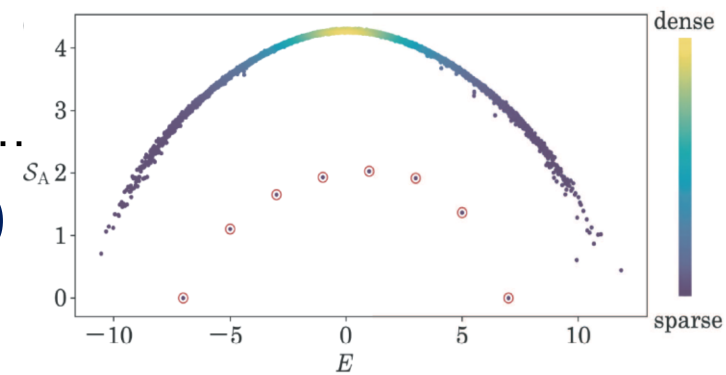


◆ Katsura, Schuricht, and Takahashi, *Phys. Rev. B* **92** (2015).

◆ Sannomiya and Katsura, *Phys. Rev. B* **99** (2019).

■ Non-ergodic quantum dynamics

- Typical non-ergodic systems
  Integrable systems, many-body localization, …



- Systems with **many-body scars (MBSs)**
  Violate eigenstate thermalization hypothesis

- Constructed models with perfect MBSs
  using Onsager algebra

◆ Shibata, Yoshioka, and Katsura, preprint (2020)