FCES19

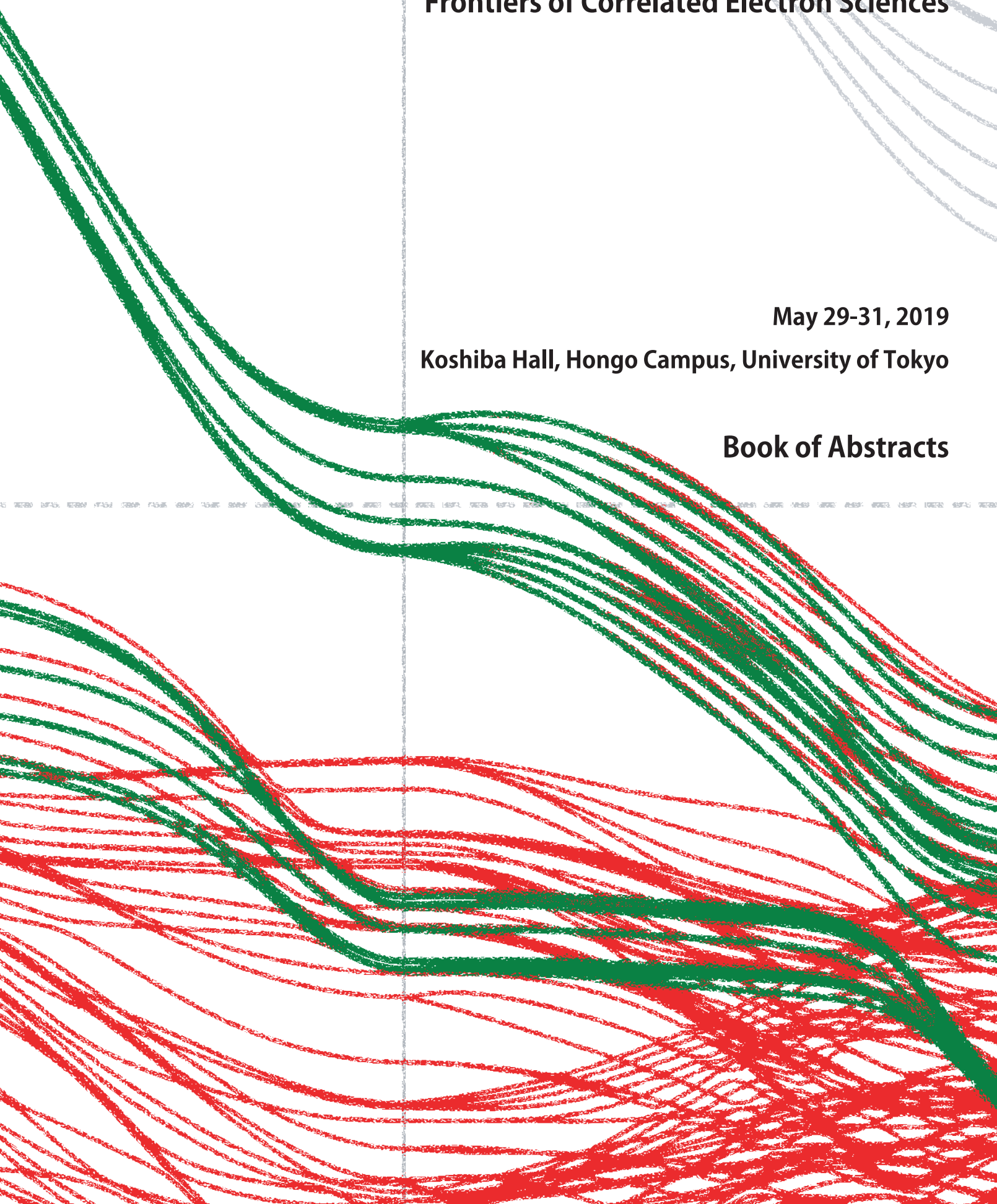
International Conference on

Frontiers of Correlated Electron Sciences

May 29-31, 2019

Koshiba Hall, Hongo Campus, University of Tokyo

Book of Abstracts

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Chair: M. Imada
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M. Imada
Closing

FCES19

International Conference on Frontiers of Correlated Electron Sciences

Date:
May 29-31, 2019

Venue:
Koshiba Hall, Hongo Campus, University of Tokyo

Scope:
This conference (FCES19) will highlight recent advances in sciences of strongly correlated electron systems and complex quantum matter. The aim of the conference is to provide a platform for members of the community in correlated electron and quantum complex matter researches including approaches with theoretical, and computational tools for new horizons of experimental developments. We encourage report on latest results, exchange information and ideas, and foster collaborations. The conference will cover the following topics:

- High-T_c superconductors including cuprate, iron-based and organic superconductors.
- Topological materials
- Efficient and functional materials such as strong permanent magnets, solar cells and thermoelectric materials
- Non-periodic systems such as thin films and interfaces as well as quasicrystals
- Nonequilibrium phenomena
- Computational methods including first-principles and correlated electron tools
- Metal-insulator transitions
- Competing orders
- Quantum criticality
- Quantum spin liquids and topological order in frustrated systems

Organizers:
Yukitoshi Motome (co-chair), Ryotaro Arita (co-chair), Takashi Miyake, Synge Todo, Shiro Sakai, and Masatoshi Imada

Sponsored by:

- "Materials Design and Exploration of Functions for Strongly Correlated Materials - topological quantum criticality, quantum multi-Challenges to Non-Equilibrium and Non-Periodic Systems –", Grant-in-Aid for Scientific Research S from Japan Society for the Promotion of Science.
- CDMSI: "Creation of new functional devices and high-performance materials to support next-generation industries", social and scientific priority issue to be tackled by using post-K computer from MEXT, Japan.

Wireless LAN:

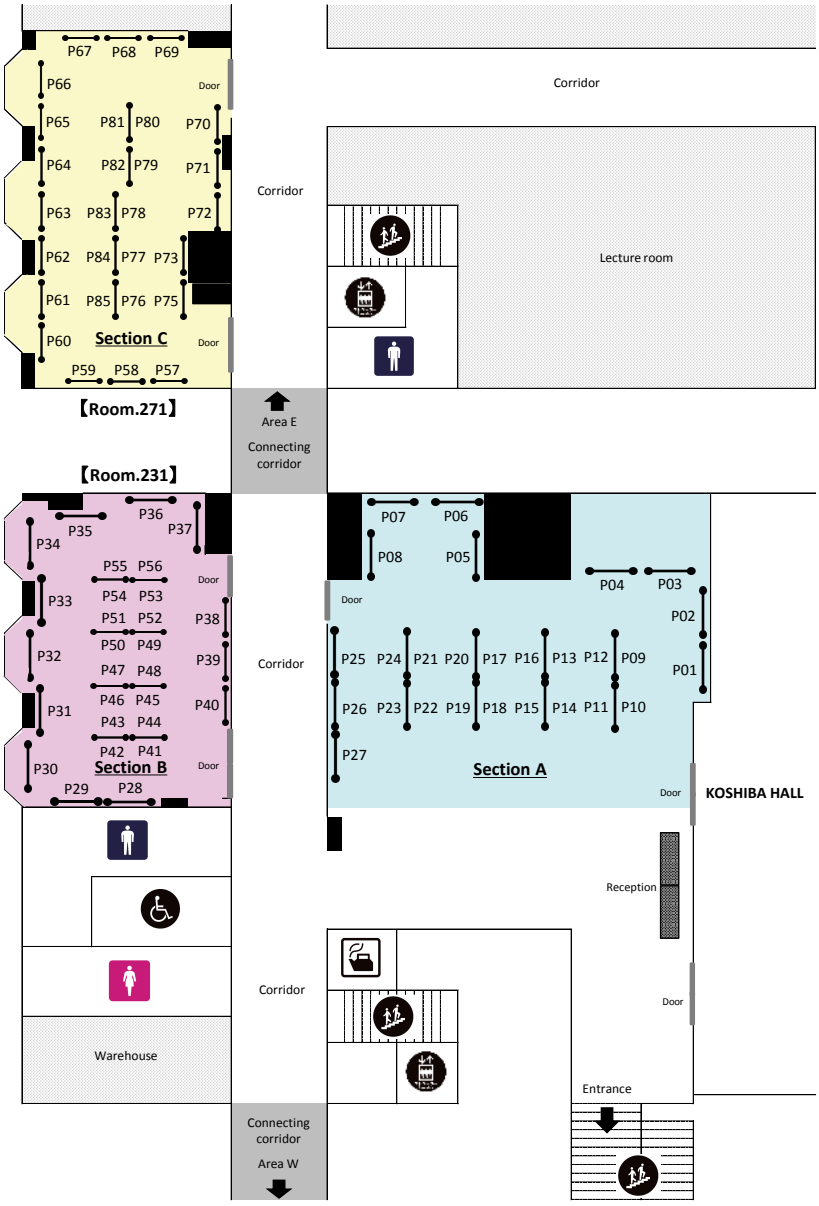
Eduroam and UTokyo-Guest can be used in the conference rooms. Detailed instruction for making registration for UTokyo-Guest is available at the reception.

Tips for Oral Presentation:

Please be advised that each presentation is followed by 5min for discussion. Please leave enough time for discussion.

Tips for Poster Presentation:

Presentation time is from 17:00 to 18:40 on May 30. The poster session will be held in parallel in three sections: section A (P01-P27, lobby of Koshiba Hall), section B (P28-P56, room 231), section C (P57-P85, room 271). *Display time* of the posters is from 14:00 on May 29 to 10:30 on May 31. Please put your poster on the poster board between 12:30-14:00 on the first day, and remove it before 11:00 on the third day at the latest.



Oral Presentations - Wednesday, May 29

9:00 - 9:10 Opening

Chair : Masatoshi Imada

9:10 - 9:40 **Gabriel Kotliar** (*Brookhaven National Labo.* / *Physics Dept., Rutgers Univ.*)
Theory of Normal State and Superconductivity in Iron Pnictides and Chalcogenides.

9:45 - 10:15 **Ivan Božović** (*Brookhaven National Labo.* / *Applied Physics Dept., Yale Univ.*)
What Makes Cuprate Superconductors so Exceptional?

10:20 - 10:35 **Takahiro Misawa** (*Institute for Solid State Physics, Univ. of Tokyo*)
Development of many-variable variational Monte Carlo method (mVMC) and its applications to high-T_c cuprates

10:40 - 11:00 Coffee Break

Chair : Fakher Assaad

11:00 - 11:20 **Atsushi Fujimori** (*Dept. of Physics, Univ. of Tokyo*)
Origin of the pseudogap in electron-doped and hole-doped cuprates revealed by ARPES

11:25 - 11:45 **Marcello Civelli** (*Laboratoire de Physique des Solides, Univ. Paris-Sud*)
A Cluster Dynamical Mean Field Theory Perspective on the pseudogap of cuprates: correlation and competition with the high T_c superconductivity

11:50 - 12:05 **Shiro Sakai** (*Center for Emergent Matter Science, RIKEN*)
Direct relation between electronic structures of Mott insulator and of high-temperature superconductor

12:10 - 12:25 **Youhei Yamaji** (*Dept. of Applied Physics, Univ. of Tokyo*)
Hidden self-energy structures of high-temperature superconductivity

12:30 - 12:50 Group photo

12:50 - 13:55 Lunch

Chair : Roser Valenti

13:55 - 14:25 **Ferdi Aryasetiawan** (*Mathematical Physics, Lund University*)
Multi-Tier Self-Consistent GW+EDMFT Scheme

14:30 - 14:45 **Kazuma Nakamura** (*Dept. of Basic Sciences, Kyushu Institute of Technology*)
RESPACK: Ab initio software for many-body perturbation calculation and effective-model derivation

14:50 - 15:05 **Claude Ederer** (*Materials Theory, ETH Zurich*)
Metal-insulator transitions in complex oxide thin films and heterostructures from DFT+DMFT

15:10 - 15:30 **Shinji Tsuneyuki** (*Dept. of Physics* / *Institute for Solid State Physics, Univ. of Tokyo*)
Transcorrelated method: the idea and its applications

15:35 - 15:55 Coffee Break

Chair : Silke Biermann

15:55 - 16:25 **Karsten Held** (*Institute for Solid State Physics, TU Wien*)
π-tons - generic optical excitations of correlated systems

16:30 - 16:50 **Yoshiteru Maeno** (*Dept. of Physics, Kyoto Univ.*)
Non-Equilibrium Steady States (NESS) of a Mott-Anderson Insulator Candidate

16:55 - 17:15 **Frank Lechermann** (*Institut für Theoretische Physik, Univ. Hamburg*)
Doping effects in the strongly correlated vanadium oxides V_2O_3 and VO_2

17:20 - 17:35 **Ryotaro Arita** (*Dept. of Applied Physics, Univ. of Tokyo* / *RIKEN Center for Emergent Matter Science*)
Cluster multipole dynamics in non-collinear antiferromagnets

Oral Presentations – Thursday, May 30

Chair : Karsten Held

9:00 - 9:30 **Antoine Georges** (*Center for Computational Quantum Physics, Collège de France / Flatiron Institute*)
Strong Correlations in Multi-Orbital Materials: Beyond Mottness.

9:35 - 9:55 **Shik Shin** (*Institute for Solid State Physics, Univ. of Tokyo*)
Topological superconductors and Multiple topological states in iron-based superconductors

10:00 - 10:20 **Yuji Matsuda** (*Dept. of Physics, Kyoto Univ.*)
Quantum oscillations and charge-neutral fermions in an insulator

10:25 - 10:40 **Sergey Streltsov** (*Institute of Metal Physics, Russian Academy of Science*)
Spin-orbit-entangled j_{eff} =1/2 state in 3d transition metal oxide: $CuAl_2O_4$

10:45 - 11:10 Coffee Break

Chair : Naoki Kawashima

11:10 - 11:40 **Silke Biermann** (*Ecole Polytechnique*)
Spectral properties of Sr_2IrO_4

11:45 - 12:00 **Takashi Miyake** (*CD-FMat, AIST*)
Magnetocrystalline anisotropy of rare-earth magnets

12:05 - 12:20 **Arun Paramekanti** (*Univ. of Toronto*)
Skyrmions: Classical spin crystals and chiral quantum liquids

12:25 - 12:40 **Toru Sakai** (*Graduate School of Material Science, Univ. of Hyogo* / *QST SPring*-8)
Spin Nematic Liquid of Low-Dimensional Quantum Antiferromagnets

12:45 - 14:05 Lunch

Chair : Gabriel Kotliar

14:05 - 14:35 **Philipp Werner** (*Dept. of Physics, Univ. of Fribourg*)
GW+DMFT simulation of lattice models in and out of equilibrium

14:40 - 15:00 **Stefan Kaiser** (*Max-Planck Institute for Solid State Research* / 4*th Physics Institute, Univ. of Stuttgart*)
Higgs Spectroscopy in Unconventional Superconductors

15:05 - 15:25 **Takami Tohyama** (*Dept. of Applied Physics, Tokyo Univ. of Science*)
Characterization of photoexcited states in the half-filled one-dimensional extended Hubbard model by machine learning

15:30 - 15:50 Coffee Break

Chair : Philipp Werner

15:50 - 16:10 **Ryo Shimano** (*Cryogenic Research Center and Dept. of Physics, Univ. of Tokyo*)
Dynamical control of superconducting order parameter by light

16:15 - 16:30 **Kenji Yonemitsu** (*Dept. of Physics, Chuo Univ.*)
Photoinduced Charge Oscillations in Correlated Dimer Systems

16:35 - 16:55 **Norio Kawakami** (*Dept. of Physics, Kyoto Univ.*)
Non-Hermitian quantum phenomena in correlated systems

17:00 - 18:40 **Poster session**

Oral Presentations – Friday, May 31

Chair : Takami Tohyama

9:00 - 9:30 **Roser Valenti** (*Institut für Theoretische Physik, Goethe-Univ. Frankfurt*)
Field- and Pressure-induced phases in generalized Kitaev models and materials

9:35 - 9:50 **Yukitoshi Motome** (*Dept. of Applied Physics, Univ. of Tokyo*)
Majorana signatures in proximate Kitaev spin liquids

9:55 - 10:10 **Peter Prelovsek** (*J. Stefan Institute, Ljubljana, Slovenia* / *Faculty of Mathematics and Physics, Univ. of Ljubljana*)
Spin liquid in extended Heisenberg models on triangular lattice

10:15 - 10:30 **Synge Todo** (*Dept. of Physics / Institute for Solid State Physics, Univ. of Tokyo*)
Optical bistability in a quantum low photon-density regime

10:35 - 11:00 Coffee Break

Chair : Norio Kawakami

11:00 - 11:30 **Fakher Assaad** (*Institut für Theoretische Physik und Astrophysik, Univ. Würzburg*)
Intertwined orders in Dirac Fermions

11:35 - 11:55 **Giorgio Sangiovanni** (*Institut für Theoretische Physik und Astrophysik, Univ. of Würzburg*)
First-order topological phase transitions with correlated electrons

12:00 - 12:20 **Yoshihiro Iwasa** (*Dept. of Physics and QPEC, Univ. of Tokyo* / *RIKEN Center for Emergent Matter Science*)
Superconductivity in 2D Materials

12:25 - 12:40 **Tomi Ohtsuki** (*Physics Division, Sophia Univ.*)
Phase Diagrams and Scaling Behaviors of Disordered Weyl Semimetals

12:45 - 13:55 Lunch

Chair : Antoine Georges

13:55 - 14:25 **Matthias Troyer** (*Microsoft Quantum*)
The Quantum Computing Future of Strongly Correlated Electron Simulations

14:30 - 14:50 **Naoki Kawashima** (*Institute for Solid State Physics, Univ. of Tokyo*)
Tensor Network States for Lattice Systems

14:55 - 15:10 **Yusuke Nomura** (*Dept. of Applied Physics, Univ. of Tokyo*)
Machine learning for solving quantum many-body Hamiltonians

15:15 - 15:45 **Masatoshi Imada** (*Waseda Research Institute for Science and Engineering, Waseda Univ.* / *Toyota Physical and Chemical Research Institute*)
Perspectives on descriptions of correlated electron phenomena

15:50 - 16:00 Closing

Poster Presentations – Section A (lobby of Koshiba Hall)

Presentation time: from 17:00 to 18:40 on May 30

Display time: from 14:00 on May 29 to 10:30 on May 31

P01 **Yuji Aoki**

Nonmetallicity in self-doped BiS_2-based $Eu_3Bi_2S_4F_4$: single crystal study

P02 **Hiromu Araki**

Higher order topological phases of a disordered breathing Kagome model: A machine learning study

P03 **Padmanabhan Balasubramanian**

Investigations on double perovskites Pr_2MnNiO_6 and $Nd_{2-x}Sr_xMnNiO_6$: Spectroscopy and *ab-initio* studies

P04 **Maxime Charlebois**

Density of states in variational Monte Carlo

P05 **Naoya Chikano**

Analysis of basic properties of compact representation of many-body Green's function

P06 **Hiroyuki Deguchi**

Chiral-Glass Phase in a Ceramic $YBa_2Cu_3O_7$ Superconductor at Low Magnetic Field

P07 **Jean Baptiste Fankam Fankam**

Electronic structure, chemical reactivity and optoelectronic properties of 4',5'-dibromo-2',7'-dinitro-3-oxo-3h-spiro[2-benzofuran-1,9'- xanthene]-3',6'-diolate from first principles calculations

P08 **Makoto Hagiwara**

Singular *I-V* characteristics in the intermediate state of intergrain ordering of a ceramic superconductor system found by a new measuring technique

P09 **Imre Hagymasi**

Dynamical topological quantum phase transitions in nonintegrable models

P10 **Hiroki Hanate**

Study on Harmonic Response and Phonon Dispersion with Inelastic X-Ray Scattering in the Geometrically Frustrated Iridate $Ca_5Ir_3O_{12}$

P11 **Kenji Harada**

Tensor network approach to non-equilibrium systems

P12 **Takumi Hasegawa**

Raman scattering investigation on geometrically frustrated iridate $Ca_5Ir_3O_{12}$

P13 **Michihiro Hirata**

Pressure-tuned velocity renormalization and excitonic fluctuations of 2D massless Dirac fermions in an organic conductor

P14 **Motoaki Hirayama**

Effective Hamiltonian for cuprate superconductors derived from multi-scale *ab initio* scheme with level renormalization

P15 **Max Hirschberger**

Skyrmion formation and enhanced emergent electrodynamics in centrosymmetric magnets

P16 **Li Huang**

Combining density functional theory with dynamical mean-field theory: Applications to the correlated actinide materials

P17 **Kota Ido**

Laser-controlled superconductivity in correlated electron systems

P18 **Shoma Iimura**

Mechanism of unconventional full-gap superconductivity in Kondo lattice with semi-metallic conduction bands

P19 **Akihiko Ikeda**

Search for excitonic condensation in $LaCoO_3$ induced at ultrahigh magnetic fields

P20 **Fumihiro Imoto**

Development of Orbital-Free Density Functional Theory with Machine Learning

P21 **Hiro Ishizuka**

Optical rectification of spin current in magnetic insulators

P22 **Ryuta Iwazaki**

Nature of superconducting fluctuation in photo-excited systems

P23 **Harald O. Jeschke**

Chromium breathing pyrochlores as a showcase for a variety of pyrochlore Hamiltonians

P24 **Ryosuke Kadono**

Metallic Spin Liquid-like Behavior of LiV_2O_4

P25 **Ryui Kaneko**

Tensor network approach to the Kitaev spin liquid

P26 **Naoyuki Katayama**

Liquid dynamics of orbital molecules with long correlation length in layered $LiVS_2$

P27 **Takeo Kato**

Quantum Critical Phenomena in Heat Transport via a Qubit

Poster Presentations – Section B (room 231)

Presentation time: from 17:00 to 18:40 on May 30

Display time: from 14:00 on May 29 to 10:30 on May 31

P28 **Harukazu Kato**

Microscopic Investigation of a phase transition between an insulator $CaCu_3Ti_4O_{12}$ and a metal $CaCu_3Ru_4O_{12}$: Cu-NQR in $CaCu_3Ti_{4-x}Ru_xO_{12}$

P29 **Kohei Kawabata**

Topological classification of non-Hermitian insulators and superconductors

P30 **Aaram J. Kim**

Spin and charge correlations across the extended pseudogap regime in the half-filled 2d Hubbard model

P31 **Akito Kobayashi**

Electronic States in Organic Conductor α-$(BETS)_2I_3$

P32 **Akihiro Koda**

Coupled Spin-Charge Fluctuation in the Semimetal Phase of All-In/All-Out Antiferromagnet $Cd_2Os_2O_7$

P33 **Koji Kudo**

Correlated higher-order topological insulator on kagome lattice

P34 **Daichi Manabe**

Supercurrent generation by spin-twisting itinerant motion of electrons in a model for cuprate superconductors

P35 **Muhamad Nasruddin Manaf**

Electron Correlation in the Anomalous Muonium in Silicon

P36 **Yasuhiro H. Matsuda**

Magnetic-field-induced insulator-metal transition in W-doped VO_2

P37 **Munehisa Matsumoto**

Doping a rare-earth permanent magnet: *ab initio* studies on the impacts in multiple energy scales

P38 **Tetsuya Minakawa**

Low-energy effective models of spin-*S* anisotropic Kitaev models

P39 **Masahito Mochizuki**

Theoretical Study on the Magnetism-Driven Negative Thermal Expansion Phenomenon in the Inverse-Perovskite Antiferromagnets

P40 **Katsuhiro Morita**

Ground-state phase diagram of the Kitaev-Heisenberg model on a kagome lattice

P41 **Yuichi Motoyama**

DSQSS – PIMC solver for quantum lattice model

P42 **Hideaki Murase**

Real-space observation of electronic crystallization

P43 **Makoto Naka**

Organic antiferromagnet as a spin current generator

P44 **Joji Nasu**

Non-equilibrium dynamics of fractional excitations in Kitaev spin liquids

P45 **Takahiro Ohgoe**

Ab initio studies on superconductivity and inhomogeneity in Hg-based cuprate superconductor

P46 **Takahiro Ohgoe**

Resummation of diagrammatic series with zero convergence radius for the unitary Fermi gas

P47 **Daigo Ohki**

Effect of Coulomb Interaction in Seebeck Coefficient of Organic Dirac Electron System α-(BEDT-TTF)$_2$I$_3$

P48 **Rikuto Oiwa**

Time-reversal symmetry breaking superconductivity in hole-doped monolayer MoS_2

P49 **Shun Okumura**

Spin-charge coupled phenomena in a chiral soliton lattice

P50 **Shun Okumura**

Numerical study of magnetic hedgehog crystals in itinerant chiral magnets

P51 **Seishiro Ono**

Symmetry Indicators for Topological Superconductors

P52 **Shota Ono**

Anomalous energy transfer between electrons and phonons in photoexcited metals

P53 **Junya Otsuki**

Strong-coupling formula of momentum-dependent susceptibilities in dynamical mean-field theory

P54 **Robert Peters**

Quantum oscillations in topological Kondo insulator

P55 **Rico Pohle**

Quantum spin liquids in the pyrochlore S=1/2 Heisenberg model with Dzyaloshinskii-Moriya interactions

P56 **Sarita Rajput**

The role of exchange interactions on spin reorientation transition of $Nd_{0.5}Dy_{0.5}FeO_3$: A first principle study

Poster Presentations – Section C (room 271)

Presentation time: from 17:00 to 18:40 on May 30

Display time: from 14:00 on May 29 to 10:30 on May 31

P57 **Panch Ram**

Inversion and Magnetic Quantum Oscillations in Kondo Insulators

P58 **Roman Rausch**

Dynamics of the magnetic polaron

P59 **Shiro Sakai**

Superconductivity in quasiperiodic systems

P60 **Tatsuki Sato**

Magneto-optic study of thermally driven ferrimagnet-helimagnet transition in a chiral-polar magnet

P61 **Thomas Schäfer**

Quantum Criticality in the Two-Dimensional Periodic Anderson Model

P62 **Makoto Shimizu**

Two-dome superconductivity in FeS induced by a Lifshitz transition

P63 **Hiroshi Shinaoka**

Dynamical susceptibility in DMFT: a sparse QMC sampling approach

P64 **Kazuya Shinjo**

Machine learning study of photoexcited states in the half-filled one-dimensional extended Hubbard model

P65 **Hiroaki Shishido**

Possible Enhancement of Coercivity in Rare-Earth Permanent Magnets on the Verge of a Valence Transition

P66 **Seiichiro Suga**

Quantized Excitation Spectra by Confinement in (Quasi-)One-Dimensional S=1 Quantum Spin Systems

P67 **Takuya Susa**

Topological Transition in Hard-Core Bosonic Haldane Model

P68 **Hidemaro Suwa**

Large-scale dynamical simulation of Hubbard model

P69 **Takafumi Suzuki**

Ground-state phase diagram of the extended Kitaev-Γ model on a honeycomb lattice

P70 **Kohei Suzuki**

Superconducting fluctuations in S=1 one-dimensional Kondo lattice model under transverse magnetic fields

P71 **Terumasa Tadano**

Ab initio derivation of effective Hamiltonian for $La_2CuO_4/La_{1.55}Sr_{0.45}CuO_4$ heterostructures

P72 **Takehiro Tani**

Field-Angle Dependence of Interlayer Magnetoresistance in Organic Dirac Electron System

P73 **Masaki Tezuka**

Characterization of quantum chaos by two-point correlators

P74 *Canceled*

P75 **Naoto Tsuji**
Spin freezing crossover and SYK strange metal

P76 **Masafumi Udagawa**
Dynamics of fractional excitations in quantum spin ice

P77 **Kentaro Ueda**
Topological phase transitions induced by pressure, band-filling, and magnetic field in strongly-correlated pyrochlore iridates

P78 **Mizuki Urai**
Disorder-enhanced quantum fluctuations in a quasi-two-dimensional organic Mott system

P79 **Alena Vishina**
High-throughput search for rare-earth-free permanent magnets

P80 **Kodai Wakamatsu**
Thermoelectric effects in a doped spin liquid candidate κ-$(ET)_4Hg_{2.89}Br_8$

P81 **Hiroshi Watanabe**
Two Competing Superconducting Phases in Molecular Conductors κ-$(BEDT\text{-}TTF)_2X$

P82 **Masahiko G. Yamada**
Theory of Proton-Driven Quantum Spin-Dipole Liquids

P83 **Kazuki Yamamoto**
Phase transitions in non-Hermitian fermionic superfluidity under complex-valued interactions

P84 **Tsuneya Yoshida**
Non-Hermitian perspective of strongly correlated systems

P85 **Nobuyuki Yoshioka**
Constructing Neural Stationary States for open quantum many-body systems

Oral Presentations – Wednesday, May 29

Theory of Normal State and Supercondctivity in Iron Pnictides and Chalcogenides.

Gabriel Kotliar

Brookhaven National Laboratory, Upton NY 11973, USA
and
Physics Department Rutgers University, Piscataway NJ 08540 USA

Hund metals are systems which derive their correlations from the Hund rule coupling rather than the Hubbard U. Primary examples are the iron pnictides and chalcogenides and the ruthenates.
In this talk I will describe recent progress in understanding this class of materials using Dynamical Mean Field Theory and advanced quantum impurity solvers. We will stress in which way Hund correlations are different from those of materials near a Mott insulating state[1]. We will conclude on how the normal state characteristics of Hund metals impact their superconducting states at lower temperatures[2].

[1] Deng et. al. arXiv:1708.05752
[2] Lee et. al. Phys. Rev. Lett. 121, 187003 (2018)

What Makes Cuprate Superconductors so Exceptional?

Ivan Božović

Brookhaven National Laboratory, Upton NY 11973, USA
Applied Physics Department, Yale University, New Haven, CT 06520, USA

An account will be given of a very comprehensive experiment in which over 2,000 single-crystal LSCO films were grown by molecular beam epitaxy and studied over the course of 12 years. The key parameters of the normal and superconducting states — ρ, R_H, magnetoresistance, T_c, λ, ξ — have been measured precisely as a function of temperature T (down to 300 mK), magnetic field B (up to 90 T), doping, and in-plane azimuth angle ϕ. [1]

The key findings are as follows. (i) The superconducting phase stiffness is extremely low, comparable to T_c. (ii) The superfluid density $N_s(T)$ decreases linearly with T, up to T_c. (iii) T_c scales with N_{s0} linearly but with an offset, except very close to the dome edges where it scales as $\sqrt{N_{s0}}$. (iv) The superconducting state develops from an electronic nematic state that breaks the $\mathbf{C_4}$ symmetry of the underlying crystal lattice. (v) The electron fluid behaves as if it were comprised of two components, one Fermi-liquid (FL) like and the other showing ρ linear in T and B; the later component diminishes and disappears with increased doping, together with the nematicity, N_{s0}, and T_c.

The related results of other groups show that the above appears to be typical of HTS cuprates and independent on the details of the Fermi surface, the number of CuO_2 planes in the unit cell, the presence or absence of CuO chains, the density and the nature of dopants, the superconducting gap size, and even whether the cuprate is underdoped or overdoped.

We conclude that HTS in cuprates involves some new physics, beyond the standard FL-BCS description. It seems to entail strong pairing, strong electron correlations, strong thermal phase fluctuations, and probably strong pair-breaking, intrinsic but T- and doping-dependent. Impurities and disorder are probably not essential, at least in the first cut.

These are just some broad conceptual constraints; much tighter ones are imposed by the particular surfaces in the (T,x,B,ϕ) space depicted by ρ, R_H, N_s, etc., which encode a wealth of incisive information about the physics of HTS, and may provide a new impetus to the theory.

[1] *Nature* **547**, 432 (2017); **536**, 309 (2016); **472**, 458 (2011); **455**, 782 (2008); **422**, 873 (2003). *Science* **361**, 479 (2018); **326**, 699 (2009); **316**, 425 (2007); **297**, 581 (2002). *Nature Materials* **12**, 877 (2013); **12**, 387 (2013); **12**, 1019 (2013); **12**, 47 (2013); **11**, 850 (2012). *Nature Physics* **10**, 256 (2014); **7**, 298 (2011). *Nature Nanotechnology* **9**, 443 (2014); **5**, 516 (2010). *Nature Communications* **2**, 272 (2011). *Phys. Rev. Letters* **106**, 237003 (2011); **102**, 107004 (2009); **101,** 247004 (2008); **93**, 157002 (2004); **89**, 107001 (2002). *Proc. Nat. Acad. Sci.* **113**, 4284 (2016); **107**, 8103 (2010).

Development of many-variable variational Monte Carlo method (mVMC) and its applications to high-T_c cuprates

T. Misawa[1], K. Yoshimi[1], M. Kawamura[1], S. Morita[1], Y. Motoyama[1], T. Ohgoe[2], K. Ido[1], M. Imada[2], and T. Kato[1]

[1]*Institute for Solid State Physics, The University of Tokyo, Japan*

[2]*Department of Applied Physics, The University of Tokyo, Japan*

High-accuracy analyses of theoretical models for quantum many-body systems are expected to play important roles for clarifying the nature of novel quantum phases such as high-T_c superconductivities and quantum spin liquids. Furthermore, recent theoretical progress enables us to obtain low-energy effective Hamiltonians for real materials in non-empirical ways [1]. To clarify the electronic structures of real materials and design materials that have desired physical properties, it is a crucial step to perform high-accuracy analyses on the low-energy effective Hamiltonians. Variational Monte Carlo method [2] is one of promising ways to perform the high-accuracy calculations for larger system sizes. Recent development of the theoretical method [3] and high-performance computers relaxes the limitations and biases imposed by the assumed form of the variational wave functions and enable us to perform highly-accurate calculations for the correlated electron systems [4,5].

We have developed mVMC (many-variable Variational Monte Carlo) [6,7], which is software for the highly-accurate variational Monte Carlo calculations with the simple and flexible user interfaces. For widely studied models of the correlated electron systems such as the Hubbard model, the Heisenberg model, and the Kondo-lattice model, users can perform the calculation by preparing only one input file whose length is shorter than ten lines. By preparing the additional input files, users can also treat general Hamiltonians such as the *ab initio* low-energy effective Hamiltonians. In the presentation, we will explain the basic usage of mVMC and its recent applications to the *ab initio* low-energy effective three-band (*dp*) Hamiltonians for the cuprates [8].

References.

[1] For a review, see M. Imada and T. Miyake, J. Phys. Soc. Jpn. **79**, 112001 (2010).

[2] For a review, see C. Gros, Ann. Phys. **189**, 53 (1989).

[3] S. Sorella, Phys. Rev. B **64**, 024512 (2001).

[4] D. Tahara and M. Imada, J. Phys. Soc. Jpn. **77**, 114701 (2008)

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Origin of the pseudogap in electron-doped and hole-doped cuprates revealed by ARPES

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The origin of the pseudogap in underdoped cuprates continues to be a highly debated issue until now. In this work, the s-symmetry pseudogap scenario proposed for the pseudogap of hole-doped cuprates [1] was tested for the "antiferromagnetic pseudogap" of electron-doped cuprates, and was found to well explain the pseudogaps both in the hole- and electron-doped compounds [2]. Our ARPES study [4] also indicated a signature of the rotational-symmetry breaking (i.e., nematicity) in the pseudogap phase [3], but suggests that the nematicity is a result of the pseudogap opening and not the origin of the pseudogap.

Collaboration with M. Horio, S. Nakata, T. Adachi, Y. Koike, H. Eisaki, D. Song, Y. Yoshida, S. Ideta, K. Tanaka, M. Hashimoto, D. Lu, Z.-X. Shen, S. Sakai, and M. Imada is gratefully acknowledged.

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A Cluster Dynamical Mean Field Theory Perspective on the pseudogap of cuprates: correlation and competition with the high Tc superconductivity

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A most striking feature of high-Tc cuprate superconductors is the appearance above the superconducting transition temperature of an unconventional metallic phase, known as the pseudogap. The relation between the pseudogap and superconductivity has been often at the front stage of the high-Tc debate. By exploiting cluster dynamical mean field theory on the two dimensional Hubbard Model, we establish key facts on the role played by the pseudogap on the cuprate phase diagram. We show that the pseudogap competes with a more conventional metallic phase over a wide range of the doping, interaction and frustration. This competition leads to a pseudogap-to-conventional metal transition in the high doping and strongly correlated region of the phase diagram, which is relevant for the cuprate physics. This is in particular revealed by a correlation-driven Lifshitz transition of the Fermi surface that explains the puzzling link between pseudogap and the Fermi surface topology pointed out in recent experiments. We shall focus in particular on the Raman response. In the superconducting phase, we show that the pseudogap and the superconductivity compete for the same electrons, producing an unconventional form of the superconducting pairing that involves electrons in high energy states. Also these findings produce a key hallmark, the so called “peak and dip” feature, in the Raman response. These results reveal an unprecedented relationship between the pseudogap and superconductivity, which eventually can be responsible for boosting up the Tc.

Direct relation between electronic structures of Mott insulator and of high-temperature superconductor

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The high-temperature superconductivity in copper oxides emerges when carriers are doped into the parent Mott insulator. This well-established fact has, however, eluded a microscopic explanation. Here we show that the missing link is a pole structure of electronic self-energy in the energy-momentum space. The continuous evolution of the self-energy pole with doping directly connects the Mott insulator and high-temperature superconductivity. We show this by numerically studying an extremely small doping region close to the Mott insulating phase in a standard model for cuprates, the two-dimensional Hubbard model, by means of a cluster extension of the dynamical mean-field theory [1,2].

We first identify two relevant self-energy structures in the Mott insulator; the pole generating the Mott gap and a relatively broad peak generating the so-called waterfall structure, which is another consequence of strong correlations present in the Mott insulator and has been discussed in the literature in connection with a spectral structure observed in angle-resolved photoemission spectroscopy for cuprates. We then reveal that either the Mott-gap pole or the waterfall structure (the feature at the energy closer to the Fermi level) directly transforms into another self-energy pole at the same energy and momentum when the system is doped with carriers. The anomalous self-energy yielding the superconductivity is simultaneously born exactly at this energy-momentum point. Thus created self-energy pole, interpreted as arising from a hidden fermionic excitation [3], continuously evolves upon further doping and considerably enhances the superconductivity. Above the critical temperature of superconductivity, the same self-energy pole generates a pseudogap in the normal state [3]. We thus elucidate a unified Mott-physics mechanism, where the self-energy structure inherent to the Mott insulator directly gives birth to both the high critical superconducting temperature and the pseudogap [4].

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Hidden self-energy structures of high-temperature superconductivity

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Origin of high temperature superconductors has long been a major challenge in physics. How electrons are mutually interacting is the key to identify the origin of superconductivity. We are, however, able to observe motion of electrons only after projection onto experimentally accessible degrees of freedom.

In this study, the Boltzmann machine learning [1, 2] is examined to extract physical quantities hidden in experimental data, combined with rigorous and physically sound prior knowledge. The method is applied to a small set of the angle-resolved photoemission spectroscopy (ARPES) spectra of copper oxide superconductors [3] to extract the normal and anomalous contributions in the self-energy separately, in which scattering processes among electrons are encoded. We reveal that prominent peak structures emerge both in the normal and anomalous self-energies, which are canceled in the total self-energy and hence not directly visible in experiments including ARPES. The revealed peaks make dominant contribution to the superconducting gap and hence provide the decisive testimony for the origin of the superconductivity [4]. Furthermore, the present achievement opens avenues for innovative machine-learning spectroscopy method in general.

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Multi-Tier Self-Consistent *GW*+EDMFT Scheme

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A parameter-free scheme for computing the electronic structure of real materials with moderate to strong electron correlations has been developed by merging the *GW* and extended DMFT methods [1,2]. The scheme sorts electrons according to their degree of correlations into tiers, each treated with an appropriate level of approximation. The interplay between short- and long-range correlations arising from the strong onsite and long-range Coulomb interaction is accounted for self-consistently.

The scheme is applied to study the spectral functions of the much investigated prototype of correlated metals, $SrVO_3$, as well as a closely related compound $SrMoO_3$. The long-range Coulomb interaction through self-consistency has the effects of enhancing screening of the impurity U and reduces its value significantly. The self-consistent impurity U becomes significantly smaller than the separation between the two satellite features conventionally interpreted as Hubbard bands. Analysis of the results suggests that it is more appropriate to interpret the satellites as collective charge excitations (plasmons) arising from the long-range Coulomb interaction. Indeed, in the case of $SrMoO_3$ LDA+DMFT cannot account for the satellites with a reasonable value of U. We have also studied sodium as a function of lattice constant to mimic correlations strength, in order to evaluate the range of applicability of the scheme.

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RESPACK: *Ab initio* software for many-body perturbation calculation and effective-model derivation

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I present an *ab initio* program package RESPACK [1] for many-body perturbation calculation and effective low-energy model derivation. RESPACK is possible to calculate the maximally localized Wannier function, response function with random phase approximation and related optical properties, frequency-dependent electronic interaction parameters, and the GW spectral function, etc. It supports *ab initio* band calculation codes using norm conserving pseudopotentials plus plane wave basis set, and officially supports xTAPP [2] and Quantum ESPRESSO [3] packages. An automatic generation script from these band-calculation output to input files for RESPACK is prepared. An input file for specifying calculation conditions is designed pursuing simplicity and is given in a namelist format. RESPACK has a wide application including simple metals, semiconductors, 3*d*/4*d* transition-metal compounds, organic and aromatic compounds, etc. It supports OpenMP/MPI and intel/GNU compiler environments. Interfaces to model-analysis solvers mVMC [4] and HΦ [5] are also provided; users can automatically obtain these inputs via RESPACK. For code developments, I acknowledge Yoshihide Yoshimoto, Yoshiro Nohara, Yusuke Nomura, Terumasa Tadano, Mitsuaki Kawamura, and Maxime Charlebois. For making interface with mVMC and HΦ, I thank to Takahiro Misawa, Kazuyoshi Yoshimi, and Yuichi Motoyama. I also thank to Masatoshi Imada, Ryotaro Arita, Takashi Miyake for application of RESPACK to material science.

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Metal-insulator transitions in complex oxide thin films and heterostructures from DFT+DMFT

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Emerging properties in complex oxide thin film and heterostructures can arise from a variety of different factors such as epitaxial strain, defects, electronic and structural reconstruction at interfaces and surfaces, charge transfer, or reduced dimensionality, which are extremely difficult to isolate experimentally. Here, we use realistic density functional theory plus dynamical mean-field theory (DFT+DMFT) calculations to explore how these factors affect the metal insulator transition in several early transition metal oxides. We demonstrate how the charge transfer across the interface gives rise to a quasi-two-dimensional metallic electron gas at the interface between the two prototypical Mott insulators $LaTiO_3$ and $LaVO_3$, and how the thickness of this emerging metallic layer can be tuned by epitaxial strain [1]. Furthermore, we analyze the metal-to-insulator transition observed in $CaVO_3$ thin films for decreasing film thickness [2,3]. We show that this transition is controlled by the interplay between epitaxial strain, dimensional confinement, and an enhanced crystal-field splitting in the interfacial layers [4]. Our results also highlight the current capabilities of the DFT+DMFT approach as a quantitative and predictive method for complex materials systems.

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Transcorrelated method: the idea and its applications

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The transcorrelated (TC) method first developed by Boys and Handy [1, 2] is a unique approach to correlated electrons with Slater-Jastrow-type many-body wave functions. In this method, by using similarity transformation of Hamiltonian with the Jastrow factor, Hartree-Fock-like self-consistent-field equations are derived for one-electron states, with which we can calculate band structure of periodic systems from first principles as well as the total energy. The method is also applicable to the Hubbard model if we adopt Gutzwiller wave functions.

For these years we have shown that the TC method is a useful approach to condensed matter [3-11]: it applies to metals in principle [3], computationally affordable [6,10], much improves the Hartree-Fock band structure of semiconductors [4,6,7], and is compatible with post-HF methods [5,8,9]. In this talk, I review the progress in the TC method for condensed matter including an application to a transition metal oxide [11].

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π-tons --- generic optical excitations of correlated systems

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The interaction of light with solids gives rise to new bosonic quasiparticles, with the exciton being---undoubtedly---the most famous of these polaritons. While excitons are the generic polaritons of semiconductors, we show that for strongly correlated systems another polariton is prevalent---originating from the dominant antiferromagnetic or charge density wave fluctuations in these systems. As these are usually associated with a wave vector k=(π,π,…) or close to it, we propose to call the derived polaritons π-tons. These π-tons yield the leading vertex correction to the optical conductivity in all correlated models studied: the Hubbard, the extended Hubbard model, the Falicov-Kimball, and the Pariser-Parr-Pople model, both in the insulating and in the metallic phase.

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Non-Equilibrium Steady States (NESS) of a Mott-Anderson Insulator Candidate

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DC current can be a powerful tuning parameter of the electronic states of strongly correlated electron systems in the vicinity of Mott transitions. We will preset on the novel phenomena in ruthenium oxide systems under such non-equilibrium steady states (NESS).

Under DC current, Ca_2RuO_4 with a small Mott gap exhibits semimetallic transport behavior with giant diamagnetism at low temperatures [1]. We attribute this behavior to emergent "Mott semimetal" state, in which the upper and lower Hubbard bands become tiny electron and hole pockets with light quasiparticle masses responsible for the large diamagnetism.

We then describe the NESS effects in the Mott-Anderson insulator candidate $Ca_3Ru_2O_7$. We will discuss similarities and differences of the NESS effects between these two ruthenate systems.

The results imply that in a non-equilibrium steady state (NESS) introduced by DC current, a variety of Mott insulators with small gaps may be driven into novel electronic states.

This work was done mainly in collaboration with C. Sow, R. Numasaki, S. Yonezawa, F. Nakamura, T. Oka, S. Kitamura, K. Kuroki, J. Zhang, M. Liu, A. Millis, D. Shibata, T. Yoshida, and N. Kikugawa. This work was supported by JSPS KAKENHI Nos. JP26247060, JP15H05852, and JP15K21717.

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Doping effects in the strongly correlated vanadium oxides V_2O_3 and VO_2

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Describing the realistic effects of impurity doping in strongly correlated compounds is a challenging problem. Electronic and lattice degrees of freedom, both on a local and global level come into play, demanding for a sound description of the bonding and many-body aspect on an equal footing.
We employ the combination of density functional theory (DFT) and dynamical mean-field theory (DMFT) to address the impact of point defects in Mott-critical transition-metal oxides. The efficient but still highly accurate implementation of the charge self-consistent DFT+DMFT method allows us to tackle the realistic correlation problem on a close-to-standard materials-science level.
Focus is here on the intriguing physics of the hallmark vanadates V_2O_3 and VO_2, both showing a metal-to-insulator transition (MIT) at stoichiometry with lowering temperature. The intriguing phase diagram of V_2O_3 with Cr- or Ti-doping will be discussed, elucidating the rather different doping physics of the different chemical impurities [1]. For rutile VO_2, we show the suppression of the MIT via the introduction of oxygen vacancies and clarify the underlying mechanism [2].
These studies on defect physics in strongly correlated materials are believed to be relevant also for future technological applications in view of a possible control of material properties by correlated-defect engineering.

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Cluster multipole dynamics in non-collinear antiferromagnets

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Recently, functional antiferromagnets are attracting an increasing amount of attention. In contrast with ferromagnetic devices, those using antiferromagnets have several advantages: They are robust against magnetic field perturbations, which is good for data retention. Since they do not have strong stray fields, one can integrate high-density memory. On top of those, the energy scale of antiferromagnets is usually higher than that of ferromagnets, which is convenient for ultrafast data processing.

In this talk, we propose a systematic framework to investigate spin dynamics in non-collinear antiferromagnets. Taking Mn_3Sn as a representative example, we derive an effective low energy model based on the multipole expansion of the magnetic structure, and investigate the uniform precession and the domain wall dynamics. We show that the solution for the effective model accurately reproduces the numerical calculation of the Landau-Lifshitz-Gilbert equations (Fig.1). Our results indicate that Mn_3Sn has preferable properties for applications to a racetrack memory and a spin torque oscillator, and thus, is a promising candidate for new devices by using the multipole degrees of freedom.

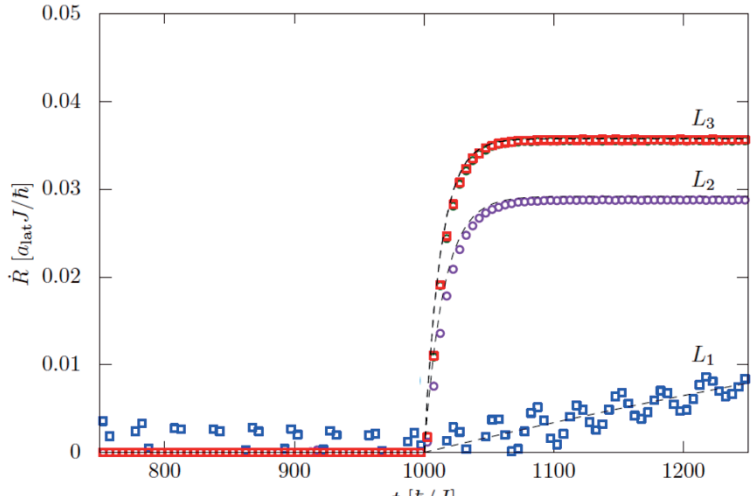

Fig. 1: Domain wall velocity as a function of time (t). Staggered magnetic field is applied for t>1000. The open squares are numerical results for a ferromagnet (blue) and collinear antiferromagnet (red). The open circles are those for Mn_3Sn. The dashed lines L_1, L_2, L_3 are analytic solutions for FM, Mn_3Sn, and collinear AFM, respectively.

Oral Presentations – Thursday, May 30

Strong Correlations in Multi-Orbital Materials: Beyond Mottness.

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Multi-band/multi-orbital materials such as transition-metal oxides, iron superconductors or twisted bilayer systems offer a fertile platform for exploring the physics of strong electronic correlations. In this context, the interplay of the `Hubbard U' with Hund's rule and spin-orbit coupling, as well as orbital differentiation, lead to rich physics beyond the paradigmatic 'Mottness'. In recent years, the concept of `Hund's metals' has emerged and has successfully explained the properties of iron superconductors and ruthenates. In this talk, I will consider mostly Sr_2RuO_4 – an amazing material which can serve as a *precision laboratory* for many-body physics. I will report on very recent high-resolution ARPES experiments [A.Tamai et al. arXiv:1812.06531] which allow to put the Dynamical Mean-Field Theory framework to a direct test, review how Hund's coupling is responsible for strong correlations in this material and emphasize the importance of spin-orbit coupling.

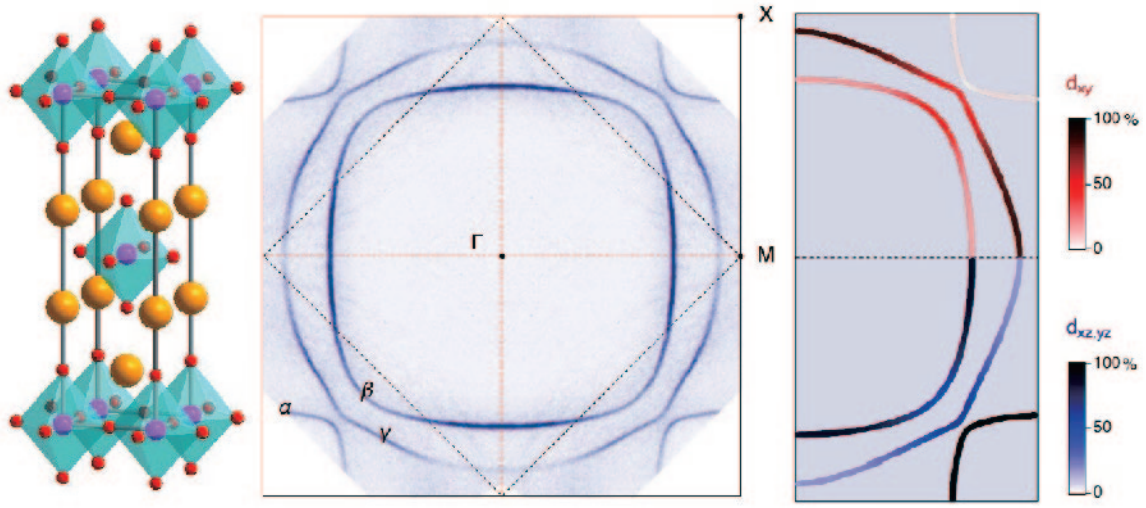

Figure credit : A.Tamai et al. arXiv :1812.06531

Topological superconductors and Multiple topological states in iron-based superconductors

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Topological materials and unconventional iron-based superconductors are both significant areas of study but, to date, relatively little overlap has been identified between these two fields. However, the combination of topological bands and superconductivity promises the manifestation of exotic superconducting states including Majorana fermions, the central component of topological quantum computation. Here, using laser-based, spin-resolved and angle-resolved photoemission spectroscopy and density functional theory calculations, we have identified both topological insulator and Dirac semimetal states near the Fermi energy in different iron-based superconducting compounds. Carrier doping can tune these topologically non-trivial bands to the Fermi energy, potentially allowing access to several different superconducting topological states in the same material. These results reveal the generic coexistence of superconductivity and multiple topological states in iron-based superconductors, indicating that this broad class of materials is a promising platform for high-temperature topological superconductivity.

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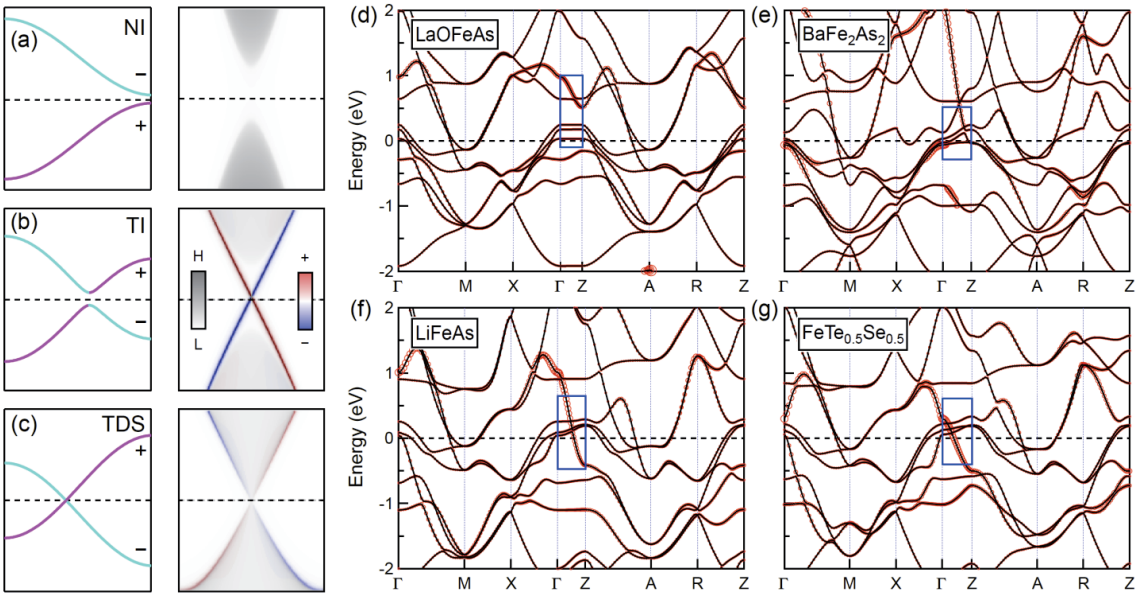

Quantum oscillations and charge-neutral fermions in an insulator

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Fermi surfaces in metallic systems can be detected by observing characteristic quantum oscillations of magnetization and electrical resistivity in a strong magnetic field--they are consequences of the quantization of the orbital motion of conduction electrons. Such oscillations, in particular of the resistivity, are absent in insulators which have no Fermi surfaces.

Here we report a profoundly controversial behavior in a Kondo insulator YbB_{12}. This material is unmistakably an insulator with an electric resistivity magnitude far beyond that of metals. However, its resistivity exhibits quantum oscillations. Analysis of the oscillations reveals the three-dimensional nature of the Fermi surface, demonstrating that the signal arises from the bulk rather than the surface. Although the oscillations of the resistivity and magnetization are observed in an insulator, their amplitude follow the conventional Fermi liquid theory of metals. The large effective masses determined by the oscillations point to the presence of Fermi surfaces consisting of strongly correlated electrons [1].

We also report the observation of gapless itinerant excitations of charge-neutral fermions in the ground state of YbB_{12} using very-low-temperature heat-transport measurements. This demonstrates that YbB_{12} is an electrical insulator but a "thermal metal". Moreover, the more insulating crystal exhibits the more metallic thermal properties, i.e., the opposite of conventional metals physics. In addition, despite the charge neutrality, the neutral fermions can couple to a magnetic field [2].

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Spin-orbit-entangled j_{eff}=1/2 state in 3d transition metal oxide: $CuAl_2O_4$

S.V. Streltsov

March 1, 2019

Spin-orbit (SO) Mott insulators are regarded as a new paradigm of magnetic materials, whose properties are largely influenced by the SO coupling and featured by highly anisotropic bond-dependent exchange interactions between the spin-orbital entangled Kramers doublets, as manifested in 5d iridates and 4d ruthenates. I will show that a very similar situation can be realized in cuprates, when the Cu^{2+} ions reside in a tetrahedral environment, like in spinel compounds. A special attention will be paid to $CuAl_2O_4$, which was experimentally found to retain cubic structure and does not show any long-range magnetic ordering down to very temperatures (0.5 K). We argue that these are the strong Coulomb correlations and the spin-orbit coupling, which conspire to suppress the Jahn-Teller distortions in $CuAl_2O_4$[1, ?]. The spin-orbit-entangled j_{eff}=1/2 state is then naturally realizes in the situation of t_{2g}^5 configuration and degenerate t_{2g} subshell. This in turn explains unusual magnetic properties of $CuAl_2O_4$. Using first-principles electronic structure calculations, we construct a realistic model for the diamond lattice of the Cu^{2+} ions in $CuAl_2O_4$ and show that the magnetic properties of this compound are largely controlled by anisotropic compass-type exchange interactions. This work was supported by Russian Science Foundation (grant 17-12-01207).

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Spectral properties of Sr_2IrO_4

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The spin orbit compound Sr_2IrO_4 has kept intriguing condensed matter scientists due to its apparent similarity to copper oxides: it is isostructural to La_2CuO_4, with a single hole in an otherwise filled t2g shell on the Ir site, and the low-energy spectrum seems well described by a single orbital degree of freedom. The pure compound is insulating at all temperatures, with antiferromagnetism setting in below 240 K. Upon doping, a metallic state is reached, which has been found to exhibit exotic (potentially cuprate-like) features.

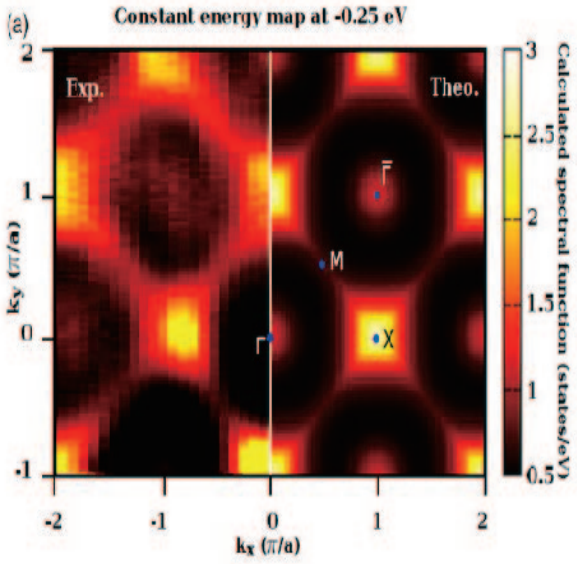

Fig. 1: Spectral function of electron-doped Sr_2IrO_4 – experiment vs. theory [3].

We will review recent advances in our theoretical modeling [1,2] of spectral properties of pure and doped Sr_2IrO_4 and related compounds, based on a novel cluster extension of dynamical mean field theory [3,4].

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Magnetocrystalline anisotropy of rare-earth magnets

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Modern high-performance permanent magnets mainly consist of 3d transition-metals and rare-earth elements. High saturation magnetization and high Curie temperature originate predominantly from interacting 3d electrons, whereas the 4f electrons play a crucial role in strong magnetocrystalline anisotropy (MCA). There is no established way of accurately calculating MCA of rare-earth magnets from first-principles, mainly because localized 4f electrons are strongly correlated [1]. In the present study, we discuss MCA of real rare-earth magnet compounds based on crystal-field theory. We will present first-principles evaluation of crystal-field parameters, and discus how chemical doping affects MCA through change in electronic states [2, 3]. We also present analysis of finite-temperature MCA using a classical spin model and constrained Monte Carlo method [4].

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Skyrmions: Classical spin crystals and chiral quantum liquids

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Motivated by recent developments in studying skyrmions in thin film ferromagnets and frustrated antiferromagnets, we discuss a triangular lattice spin model with anisotropic spin exchange interactions which hosts such noncoplanar spin crystals. We consider both ferromagnets with broken inversion symmetry which host Dzyaloshinskii-Moriya (DM) interactions, and antiferromagnets where symmetry forbids DM interactions but permits so-called "compass exchange" terms which are relevant to recent experiments on materials such as Gd_2PdSi_3 [1]. We show that nonlinear mode-mode coupling in such systems can lead to highly field tunable skyrmion crystals [2]. Finally, we present numerical results on some spin-1/2 Heisenberg models, showing how quantum fluctuations can melt skyrmion order, leading to chiral quantum spin liquids [3].

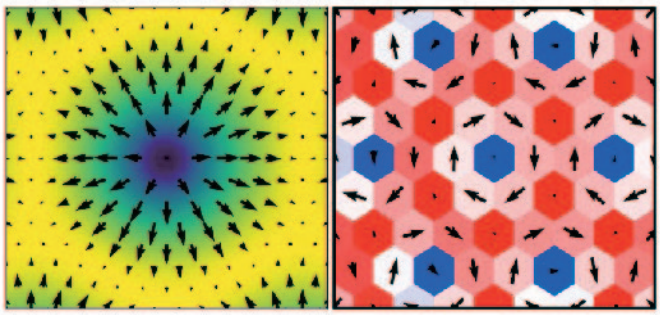

Fig. 1: Skyrmions in 2D Rashba ferromagnets and in centrosymmetric frustrated antiferromagnets

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Spin Nematic Liquid of Low-Dimensional Quantum Antiferromagnets

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The spin nematic phase, which is a kind of multipole phases, has attracted a lot of interest in the field of the strongly correlated electron systems, as well as the quantum spin liquid phase. Using the numerical exact diagonalization, the density matrix renormalization group (DMRG) calculation, and the finite-size scaling analysis, it is found that some spin nematic and spin liquid phases are induced by external magnetic field in the anisotropic and/or frustrated quantum spin systems. In our previous work[1], it was found that a field-induced nematic phase appears at some critical field in the anisotropic spin ladder and the mixed spin chain. The nematic phase is characterized by the power-law decay in the correlation function of the second-order spin moment. In addition at some higher critical field a quantum phase transition can occur to the conventional field-induced Tomonaga-Luttinger liquid. Several typical magnetization curves calculated by DMRG are presented.

Recently the field-induced nematic phase was observed on the frustrated spin ladder system[2]. So we study on a frustrated spin ladder system[3], using the numerical diagonalization and DMRG. As a result, it is found that several exotic quantum phases, including the spin-nematic liquid phase. We also report some exact eigenstates of the present model and present several interesting phase diagrams[4].

Our recent numerical diagonalization study[5] on the S=1 spin ladder system with the easy-axis single-ion anisotropy suggested that the field-induced nematic Tomonag-Luttinger liquid (TLL) phase appears. In addition another spin nematic liquid phases were predicted in the three-leg ladder system with the ring exchange interaction[6]. Some realistic candidates which possibly exhibit the spin nematic phase will be proposed.

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GW+DMFT simulation of lattice models in and out of equilibrium

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The GW+DMFT method provides a consistent scheme for the description of correlation and screening effects in lattice systems and a powerful tool for the study of nonequilibrium states [1,2]. We will discuss the formalism and its implementation for simple lattice models (single-orbital Hubbard and three-orbital "d-p" model) and investigate the effect of dynamical screening on the local interaction and spectral function. For the d-p model of charge transfer insulators, we demonstrate that the GW contribution to the self-energy is not relevant in equilibrium, but crucially important for the description of photo-excited states [3]. These model-level studies are a first step in the development of parameter-free ab-initio simulation approaches for correlated materials.

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Higgs Spectroscopy in Unconventional Superconductors

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The complex phase diagram of cuprate high-Tc superconductor is due to an intriguing interplay of different orders such as the pseudogap, or charge order. Despite intensive spectroscopic measurements of these ordered states, yet the microscopic mechanism behind high-Tc superconductivity is still lacking.

In particular the collective dynamics of the superconducting order parameter, the Higgs mode, was not accessible so far. Here we report on "Higgs spectroscopy" in cuprate superconductors that we accomplished by using a high-field multicycle THz pulse, which nonlinearly couples to the superconducting condensate and leads to characteristic third harmonic generation [1]. We identify the driven Higgs amplitude response of the superconducting order parameter in four archetypal families of cuprate thin films and we report on a novel collective mode universally exhibited by optimally doped samples. In addition, we find a finite Higgs-like response above Tc that might be interpreted as finite pairing amplitude even above Tc.

This remarkable example illustrates the power of Higgs Spectroscopy as novel tool to investigate the eigenmodes of coherent condensates – also beyond superconducting condensates [2] - with respect to their symmetries and possible couplings to external modes or interplay with competing or intertwined orders.

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Characterization of photoexcited states in the half-filled one-dimensional extended Hubbard model by machine learning

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Nonequilibrium processes in strongly correlated electron systems can provide new insights into the dynamical properties of these systems, which can be qualitatively different from their weakly interacting counterparts. One such example is nonequilibrium induced phase transition. As the system is driven away from the equilibrium, under certain conditions, a ‘‘crossover’’ from one state to another metastable state may occur. Such an indication has been reported theoretically in the half-field one-dimensional extended Hubbard model (1DEHM) [1], where by tuning the laser frequency and strength a sustainable charge order enhancement is found when the system is originally in the spin-density-wave (SDW) phase but close to the transition to charge-density wave (CDW). However, the detailed nature of the photoexcited state over full parameter space is still unclear.

To characterize the photoexcited states in the 1DEHM, we apply supervised machine learning [2]. We use the following procedure. Firstly, using density-matrix renormalization group (DMRG), we calculate the ground state of 1DEHM with correlated hopping terms that are suggested from the Floquet time-independent effective model of a driven Hubbard model. We next prepare entanglement spectrum (ES) for the possible ground states with SDW, CDW, bond-charge-density wave (BCDW), and bond-spin-density wave (BSDW). Using these ES, we construct neural network with four layers. Finally we use the neural network to judge the ES of photoexcitaed wave functions of the 1DEHM. Predicted phases are checked by time-dependent local and non-local correlation functions obtained by time-dependent DMRG. Using this procedure, we predict a possible BSDW for the photo-driven 1DEHM in a region of the CDW ground state and confirm this by calculating the various time-dependent correlation functions.

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Dynamical control of superconducting order parameter by light

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Optical manipulation of quantum system has gained a growing interest over decades. With the recent development of ultrafast advanced light sources, the concept is now being applicable to complex condensed matter systems with avoiding a thermalization effect at least in a transient manner. In particular in superconductors, the light-control of superconducting order parameter is a fascinating subject as it potentially elucidates the hidden phases which are inaccessible by static perturbation, and also provides deep insights into the ground sate properties in equilibrium. Toward this aim we have adopted two approaches:1) dynamical control of superconducting order parameter by light, in particular in terahertz frequency range, and 2) quenching of those orders that competes with superconductivity. Along with the first scheme, after a brief review on our recent observation of the Higgs mode, namely the amplitude oscillation of order parameter in conventional and unconventional superconductors [1-3], we report our recent investigation on its extension to a two-band superconductor $FeTe_xSe_{1-x}$. A transient enhancement of order parameter as well as the relation between the multiple order parameters will be discussed. In the second scheme, we investigated the photo-quench dynamics in a nematic phase of FeSe and in a charge density wave phase of transition-metal dichalcogenides. Nonequilibirum dynamics of those symmetry broken ground states will be discussed.

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Photoinduced Charge Oscillations in Correlated Dimer Systems

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Photoinduced phenomena in correlated electron systems are not limited to melting/ordering phase transitions (including those to hidden states) or ultrafast control of conduction/magnetism. Here we report characteristic electron dynamics that emerge only after a strong pulse of an oscillating electric field is applied.

In an organic dimer-Mott insulator/superconductor, κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br, which is known for intriguing critical phenomena, stimulated emission (i.e., increased reflectivity and transmittance at a specific energy) has been observed after a strong light pulse is applied [1]. Its energy is on the high-ω side of the linear absorption spectrum.

This is theoretically shown by exact diagonalization as due to a nonlinear charge oscillation, which is related to a discrete time crystal in many-body localized driven systems [2]. The oscillation is regarded as an electronic breathing mode [Fig. 1] and widely observed in dimerized systems. The initially uniform charge density is disproportionated inside a dimer and coherently oscillates after photoexcitation. Its frequency is expressed by all of the (i.e., both intra- and inter-dimer) transfer integrals that connect charge-rich to -poor sites. The result is consistent with the experimental results for κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br and κ-(*d*-BEDT-TTF)$_2$Cu[N(CN)$_2$]Br.

This nonlinear charge oscillation has a finite life time (for interacting systems), but its life time is longer than any charge oscillation responsible for the linear optical conductivity. In fact, the nonlinear charge oscillation becomes dominant in the Fourier spectrum as the Coulomb interaction is increased. Thus, it is regarded as interaction-induced synchronization. Because it is triggered by a pulse excitation, thermalization is avoidable, which is in contrast to a discrete time crystal.

In the experiment, the amplitude of the nonlinear charge oscillation is enhanced near the superconducting transition temperature. The effect of superconductivity is discussed using a mean field approximation. Depending on the interaction strength, different types of nonlinear charge oscillations are shown to appear [3]. For the electronic breathing mode, the result is consistent with the experiment.

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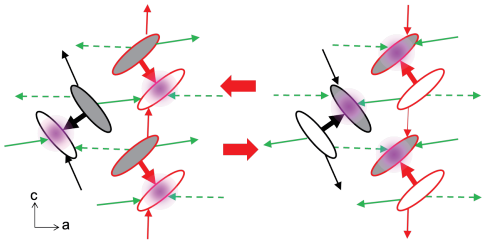

Fig. 1: Electronic breathing mode

Non-Hermitian quantum phenomena in correlated systems

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Recently, non-Hermitian quantum phenomena have attracted a great deal of attention. We here address the following two interesting issues in this context.

1. *Non-Hermitian Kondo effect* [1]: We first investigate the Kondo effect in an open quantum system motivated by recent experiments with ultracold alkaline-earth(-like) atoms. Due to inelastic collisions and the associated atom losses, this system is described by a non-Hermitian extension of the Kondo problem. We show that the non-Hermiticity induces anomalous reversion of renormalization-group, leading to a unique quantum phase transition (Fig.1). Furthermore, by exactly solving the non-Hermitian Kondo Hamiltonian, we obtain the critical line consistent with the renormalization-group flow.

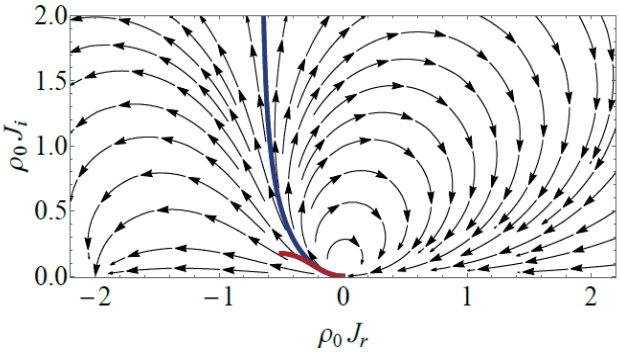

Fig. 1: RG flow of real- imaginary Kondo couplings

2. *Non-Hermitian perspective on Kondo lattice systems* [2,3]: We then address a slightly different topic: a two-dimensional Kondo lattice model in equilibrium with special emphasis on its non-Hermitian properties [2], following a recent proposal by Kozii and Fu [4]. We confirm that the single-particle spectral weight shows the exceptional points (EPs). Correspondingly, the spectral weight exhibits the band touching, resulting in a structure similar to the Fermi arc. Furthermore, we find that the paramagnetic phase in the low temperature region shows a significant difference from non-interacting fermions: the imaginary part of the self-energy yields the Fermi loop without any defective points. We extend the notion to symmetry-protected exceptional rings [3].

This work is done in collaboration with M. Nakagawa, M. Ueda, K. Takasan, T. Yoshida, R. Peters and Y. Hatsugai.

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Oral Presentations – Friday, May 31

Field- and Pressure-induced phases in generalized Kitaev models and materials

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In the search for novel materials' properties, the generation and manipulation of highly entangled quantum states is a grand challenge of solid state research. Amongst the most entangled proposed states are quantum spin liquids. In this context, the exactly solvable Kitaev Z_2 spin-liquid model, for which finely tuned anisotropic interactions exactly fractionalize spins into fermionic Majorana spinons and gauge fluxes has activated an enormous amount of interest. Most specially since possible realizations may be achieved in octahedral coordinated spin-orbit-coupled 4d5 and 5d5 insulators. However, the low symmetry environment of the known Kitaev materials also allows interactions beyond the Kitaev model that open possible new routes for further exotic excitations.

Based on *ab initio* and many-body simulations and comparison to experimental observations, we will discuss in this talk, the challenges that one faces in designing such materials and in identifying the origin of their excitations. We will further present recent results [1-6] on possible field- and pressure-induced phases obtained by adding to the Kitaev model further interaction terms and will discuss the relevance of the results in relation to honeycomb iridates and α-$RuCl_3$.

Work done in collaboration with Steve M. Winter, Kira Riedl, David Kaib, Ying Li, Andreas Honecker, Pavel A. Maksimov, Alexander L. Chernyshev and Radu Coldea

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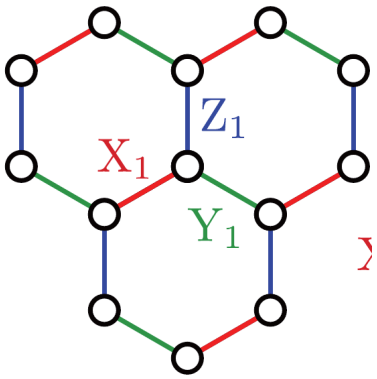

Majorana signatures in proximate Kitaev spin liquids

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A Majorana fermion is a fermionic particle that is its own antiparticle. The exotic particle has long been pursued since the proposal by Ettore Majorana in 1937. Recently, it has attracted renewed interest in condensed matter physics, where it can be realized as quasi-particles in quantum states of matter [1]. In this talk, we discuss a candidate for such realization of Majorana fermions, quantum spin liquids, where strong quantum fluctuations suppress any conventional symmetry breaking and leave the electron spins disordered but quantum entangled. In particular, we focus on the so-called Kitaev spin liquids, where the electron spins are fractionalized into Majorana fermions and Z_2 fluxes [2]. We will give an overview of our recent findings, especially focusing on the peculiar properties associated with the fractional excitations, such as thermal fractionalization [3], signature of fermionic excitations [4], dichotomy of static and dynamical spin correlations [5], and Majorana topological states in an applied magnetic field [6]. We will also discuss our recent proposals for materials exploration [7].

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Spin liquid in extended Heisenberg models on triangular lattice

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Motivated by recent experiments, revealing a spin liquid phase in the layered 1T-TaS_2 [1], we study the finite-temperature static and dynamical properties of the extended J_1-J_2 Heisenberg model [2]. Here, frustration enables to reach reliable results to considerably lower T relative to the unfrustrated lattices. Indications for the onset of spin liquid phase are visible in thermodynamic quantities, as the specific heat, but also in dynamical structure factor, being related to experimentally relevant NMR relaxation rate $1/T_1$, which can be used as the hallmark for the spin liquid. Further I will present the reduced-basis approach using the triangle as the basic unit which allows the unifying treatment of the Heisenberg models on triangular and kagome lattices. The approach enables the study of larger systems, but reveals also similarities and differences between both lattices, in particular in relation to the existence of spin-liquid regimes.

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Optical bistability in a quantum low photon-density regime

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Spins coupled with photon degrees of freedom in the cavity (Fig.1) exhibit various responses to the incident laser field depending on the average number of photons in the cavity. One of the most characteristic phenomena is the dynamical first-order phase transition, in which the number of photons in the cavity shows bistability with respect to the laser intensity, and jumps discontinuously between the states. Until now, the analyses of this phenomenon have been carried out based on the mean-field treatment that becomes exact in the limit of infinite number of spins, or based on numerical simulations for small spin number in the limit of infinite number of photons. We realized a large-scale simulation utilizing the parallelization with respect to the photon number and the symmetry of the spin state, and examined the size dependence of the photon number distribution and the relaxation time in the low photon-density regime from the eigenvalues and eigenstates of the time evolution operator. We show that in the low photon density regime the laser frequency dependence of the metastable state is qualitatively different from that in previous studies, and discuss the optical bistability from the effective free-energy picture of the dynamical first-order phase transition. Furthermore, we calculate the hysteresis loop (Fig.2), which appears when the laser intensity is periodically modulated, from the viewpoint of the Floquet operator, and clarify that a dynamical phase transition phenomenon appears with respect to the period of modulation.

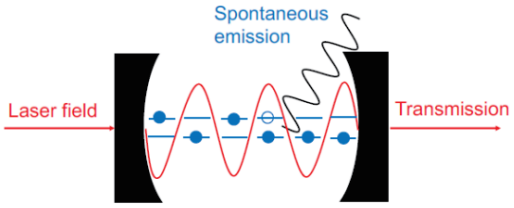

Fig. 1: Spins in the cavity.

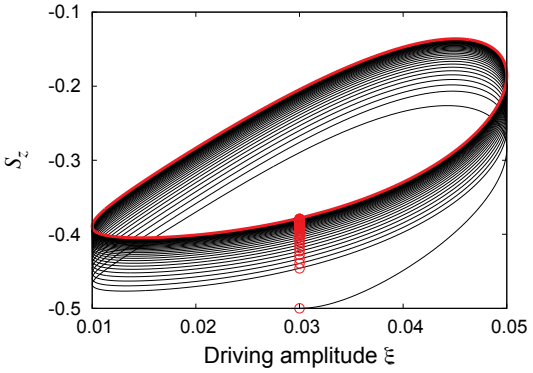

Fig. 2: Hysteresis loop and limit cycle under periodic modulation of laser intensity.

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Intertwined orders in Dirac Fermions

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There has recently been a flurry of negative sign free fermionic models that exhibit exotic phases and phase transitions. After reviewing these advances, I will place the emphasis on models of Dirac fermions in 2+1 dimensions with dynamically generated anti-commuting mass terms. For eight component Dirac fermions as realized in Graphene, one can find 56 quintuplets of anticommuting mass terms. For example the three antiferromagnetic masses and two valence bond solid ones form such a quintuplet. Another quintuplet combines the quantum spin Hall mass terms with the two s-wave superconducting ones. Here, I will present a model free of the negative sign problem that dynamically generates the quantum spin Hall and s-wave superconducting phases and show results supporting a direct and continuous phase transition between these two states [1]. More generally, we will argue that models of Dirac fermions with dynamically generated anti-commuting mass terms are a golden route to realize and investigate exotic quantum phase transitions beyond the Ginzburg-Landau-Wilson paradigm.

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First-order topological phase transitions with correlated electrons

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When the bandstructure of a topologically trivial insulator evolves into that of a quantum spin Hall, the gap closes and inverts gradually. The situation can drastically change if the electrons experience a strong Coulomb repulsion. The second-order phase transition turns into a discontinuous one and the system eschews to be fine-tuned to a gapless semimetal [1].

In this talk I am going to show that two-orbital microscopic models for two- and three-dimensional topological insulators display a first-order phase transition. This originates from the asymmetry resulting from the rapid growth of the many-body character on the non-trivial side, while the band insulator persists in its Hartree nature [1, 2]. This "blending" between non-trivial topology and local orbital physics is the key physical ingredient which allows us to define local observables diverging at the quantum critical point.

The boundary modes in the topologically non-trivial phase are influenced by the presence of the high-spin Mott insulating phase at even larger values of U. We indeed observe a boundary reconstruction in 2D: the edge states get gapped out in the outmost part of the slab and settle in sub-peripheral layers [3]. Upon allowing for time-reversal symmetry breaking this turns into an interesting coexistence of correlated metallic modes and antiferromagnetism [4].

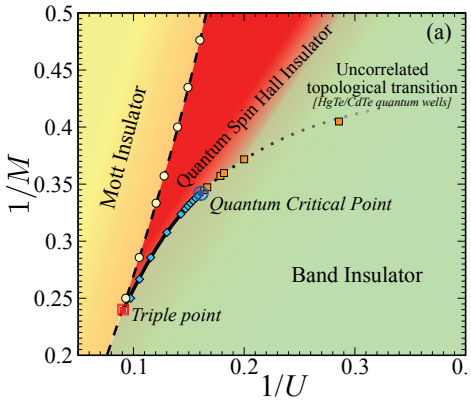

Fig. 1: Phase diagram of the Bernevig-Hughes-Zhang-Hubbard model. Taken from Ref. [1]

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Superconductivity in 2D Materials

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2D materials are a rich materials platform of designing novel properties and functions. One examples is superconductiviy in 2D materials, obtained by mechanically exfoliated mono or a few layers, heterointerfaces, electric-double-layer transistors, and molecular-beam-epitaxy grown or chemical vapor deposited atomically thin layers [1]. All these 2D superconductors have very high crystallinity in marked contrast with the conventional 2D superconductors with amorphous or granular structures, and thus provide opportunities for investigating the intrinsic nature of 2D superconductors, reflecting the high crystallinity of 2D materials. Nowadays, people are excited about the new opportunity of flatband physics and superconductivity in twisted bilayer graphene [2].

Here we review the novel aspects of highly crystalline 2D superconductors with particular focus on the gate-induced 2D superconductivity using electric double layer transistor devices. Topics include quantum metallic states (Bose metal) [3], quantum Griffiths phases [4], dramatically enhanced Chandrasekhar-Clogston-Pauli limit due to the spin-orbit interactions [5], and nonreciprocal superconducting transport [6]. Also, EDLTs was found to offer a new opportunity to control electrochemical reactions, which allows us to access superconductivity in monolayer FeSe [7] and very lightly doped superconductor in ZrNCl toward BCS-BEC crossover [8].

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Phase Diagrams and Scaling Behaviors of Disordered Weyl Semimetals

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Recent experimental discovery of Weyl semimetals stimulated extensive studies of this novel topological material. In the presence of disorder, Weyl semimetal systems show rich phase diagram: Weyl semimetal (WSM), band /Chern insulator (BI/CI), as well as diffusive metal phases. By changing the mass parameter, the system undergoes CI to WSM transition, while increasing the strength of disorder induces diffusive metal (DM) phase.

We demonstrate that the machine learning method to detect surface Fermi arc states gives reasonable phase diagram[1,2] (see Figure 1). We further show that rich unconventional scaling behaviors are expected across and on the phase boundaries.[3,4]

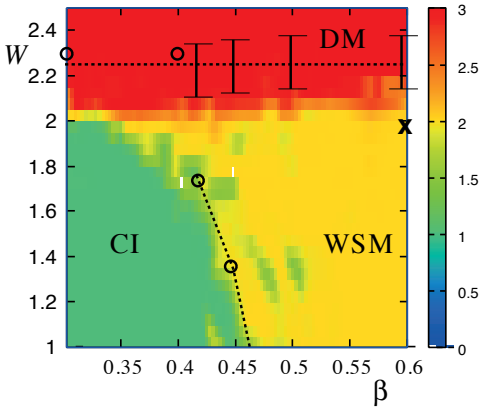

Fig. 1: Phase diagram obtained by machine learning the surface Fermi arc states. The horizontal axis β indicates the mass parameter, while the vertical axis W indicates the strength of disorder.

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The Quantum Computing Future of Strongly Correlated Electron Simulations

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The exponential complexity of simulating correlated quantum systems on computers has motivated Richard Feynman to propose that we should use computers employing quantum principles to simulate Nature. As we make progress towards scalable implementations of such quantum computers it is timely to start thinking about how we would use them to solve important problems in correlated electron science. Correlated quantum systems will be one of the most important applications of quantum computers.

In my talk I will present an overview of how quantum computers will revolutionize this field in the future. I will discuss quantum algorithms for the simulation of ground states, excited states and non-equilibrium dynamics. I will present ideas of solving the infamous negative sign problem of quantum Monte Carlo simulations on quantum computers.

I will also go into specific runtime estimates for the above simulations. We found that, despite an exponential improvement in scaling compared to classical computers the brute-force ab-initio simulation of materials and molecules is still challenging even on quantum computers. Effective models, like variants of the Hubbard model, will thus be the initial targets for quantum computers. Hybrid quantum/classical methods and embedding approaches like dynamical mean field theory will also become more powerful when accelerated with quantum computers.

I will end with a vision of how our field of research may look like in the age of quantum computing.

Tensor Network States for Lattice Systems

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While the tensor network representation has been used in variational calculations of lattice many-body problems since 1960s, it is relatively recently that the concept drew attention it deserves. In the last few decades, various efficient scheme for practical computation were devised while the connection to the analytical theories became clearer. One of the most well-known examples for the latter may be the AKLT state for the symmetry protected topological order. While it is not the ground state of the original problem, i.e., the S=1 antiferromagnetic Heisenberg chain, it captures its essence in terms of the 1D tensor network state (i.e., a matrix-product state) with only a binary degree of freedom for each virtual index. I present some tensor-network calculations [1] of the Kitaev honeycomb model, which is the exactly solvable model for topological spin liquids. Whereas no compact tensor network representation is known for the ground state of the Kitaev honeycomb model, we propose one with only binary degree of freedom as a good initial state for the variational calculation. This state satisfies most of the desirable properties that the exact ground state is known to possess. By introducing a variational parameter in the form of the tensor network operator (sometimes referred to as PEPO), we can further improve the wave function, though it increases the necessary bond dimension to 4 or larger. With the bond dimension of 8 we reach relative error of 10^{-4} (in energy) with only two tunable parameters. While these results are specialized for the Kitaev honeycomb model, they may serve as a prototype for tensor-network application to the spin liquid states.

[1] Hyun-Yong Lee, Ryui Kaneko, Tsuyoshi Okubo and Naoki Kawashima, unpublished.

Machine learning for solving quantum many-body Hamiltonians

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Department of Applied Physics, University of Tokyo

Machine learning techniques can be used to extract essential feature of quantum many-body wave functions (=vectors with exponentially large dimensions), and to obtain compact representations of many-body states. Indeed, recently, variational wave function written in terms of restricted Boltzmann machine (RBM) has been introduced to represent ground states of quantum spin Hamiltonians [1]. The RBM wave function has been shown to be able to represent ground states of spin Hamiltonians in high accuracy [1].

In the present study, we introduce efforts to improve the accuracy of RBM wave functions by i) combining concepts from machine learning and physics [2] and by ii) introducing deep Boltzmann machine (DBM) having additional hidden layer on top of the RBM structure [3].

In i), we introduce a new form of variational wave function, called RBM+PP, which combines RBM with pair-product (PP) wave functions [2]. The combined wave function can be applied not only to bosonic models but also to fermionic models. The combined method improves the accuracy beyond that ever achieved by RBM and conventional wave-function method separately, thus proving its power as an accurate solver.

In ii), we show a deterministic approach to generate deep-Boltzmann-machine (DBM) network to represent ground states of many-body Hamiltonians [3]. Thanks to more flexible representational power of DBM compared to RBM, the DBM state can reproduce the exact imaginary-time Hamiltonian evolution with the number of hidden units proportional to the system size and imaginary time, respectively. Once the network is constructed, physical quantities can be measured by sampling both the visible and hidden variables. The present construction of classical DBM network provides a novel framework of quantum-to-classical mappings (In special cases, it becomes equivalent to path-integral formalism).

The present works have been done in collaboration with Andrew S. Darmawan, Youhei Yamaji, Masatoshi Imada, and Giuseppe Carleo.

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Perspectives on descriptions of correlated electron phenomena

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and
Toyota Physical and Chemical Research Institute, Nagakute, Aichi, Japan

Strongly correlated electron systems have been a challenging and central subject in physics for decades. Emergent phenomena including exotic magnetism, unconventional transport, and superconductivity have extensively been studied as playgrounds of emergent and universal concepts of nature and as seedbeds of potential functionality for future innovative applications.

After the discovery of cuprate high-T_c superconductors, it has been widely recognized that deeper understanding of fermionic many-body systems relevant to realistic materials is required beyond conventional theoretical frameworks. Necessity of describing realistic materials representable originally by exponentially large Hilbert space has urged us to develop multi-scale *ab initio* method with downfolding, allowing correct descriptions of materials by using only low-energy degrees of freedom, which can be solved within the available computational cost by accurate low-energy solvers in the next step. High accuracy is required because of the severe competitions among various quantum phases and fluctuations, hallmark of strongly correlated systems.

Theoretical and computational methodologies have been updated and improved for more accurate and realistic descriptions for both of better downfolding procedure such as the constrained GW and more accurate solvers such as tensor network and machine learning tools. The improved scheme now allows quantitative and predictable descriptions of real correlated materials even for challenging issues including unconventional superconductivity of the cuprate and iron-based superconductors. It also inspires us to novel concepts such as spin liquids, fractionalization with emergent or dark fermions and Planckian fluids with unparticle concept. The research front is now extended also to fields such as non-equilibrium phenomena, non-periodic systems including interfaces, surfaces and random systems, and topological materials with strong correlation effects. After summarizing some of recent achievements and interesting proposals presented in this workshop, I discuss my personal view for future challenges to be tackled.

Poster Presentations – Section A

Nonmetallicity in self-doped BiS_2-based $Eu_3Bi_2S_4F_4$: single crystal study

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BiS_2-based layered materials [1] show rich variety of correlated electron physics, which are partly attributed to locally-noncentrosymmetric BiS_2 layers with strong spin-orbit coupling [2]. We have succeeded in growing single crystals and have revealed a quantum critical behaviors ($\ln T$ divergence in specific heat) in $CeOBiS_2$[3], anisotropic-gap superconductivity and the absence of a Pauli paramagnetic limit in $LaO_{0.5}F_{0.5}BiS_2$[4], and lattice instabilities $La(O,F)BiS_2$ [5]. In this presentation, we focus on $Eu_3Bi_2S_4F_4$ (see Fig. 1 for the crystal structure).

$Eu_3Bi_2S_4F_4$ has been reported to exhibit superconductivity with a transition temperature of 1.5 K using polycrystalline samples [6]. Studies using our single crystals have revealed anomalous thermodynamic and transport properties. Mixed valent Eu ions with the average valence of +2.19 indicates the self-doped electron density in BiS_2 layers to be 0.29 electrons per Bi site, which is consistent with our ARPES measurements [7]. It has been revealed, however, that the resistivity shows an anomalous nonmetallic behavior with $1/T^3$ dependence without any sign of superconductivity, in marked contrast to a metallic behavior in the polycrystals. This behavior suggests an unconventional *electron-localization mechanism* working in the single crystals, possibly caused by Eu^{2+}/Eu^{3+} distribution (or fluctuations) and/or lattice instabilities inherent to BiS_2 layers.

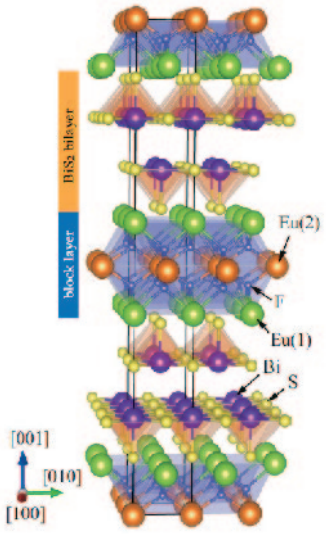

Fig. 1: Crystal structure of $Eu_3F_4Bi_2S_4$ ($I4/mmm$, #139).

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Higher order topological phases of a disordered breathing Kagome model: A machine learning study

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University of Tsukuba

A higher order topological insulator (HOTI) is a new concept of topological states of matter, characterized by the emergent boundary states whose co-dimension is higher than one. So far, several tight-binding models for HOTI are proposed [1,2], which triggered many theoretical and experimental studies. However, its robustness against disorders has not been well understood.

In this presentation, we show the phase diagram of HOTI phases in a breathing Kagome model in the presence of disorders, by using a machine learning technique [3]. We find that the corner states survive against the finite strength of disorder potential as long as the energy gap is not closed, indicating the stability of the HOTI phases against the disorders. We also discuss the relation between the HOTI phase and the Z_3 Berry phase [4], which is a bulk topological invariant.

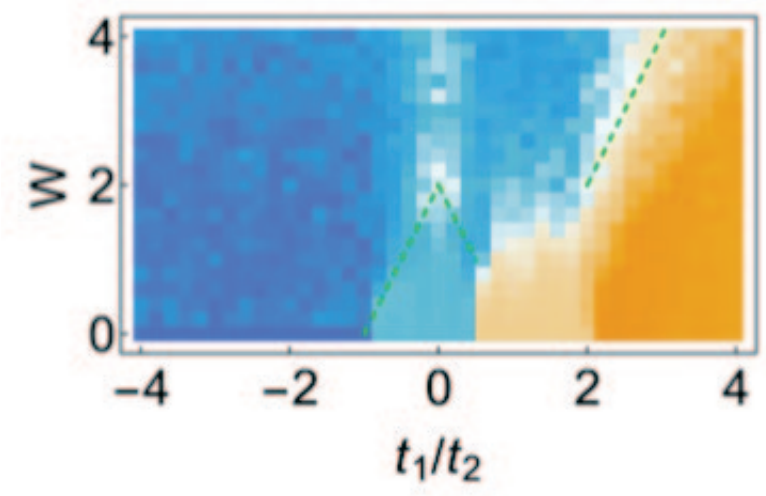

Fig. 1: Phase diagram of the breathing kagome model. Horizontal axis is the breathing parameter and the vertical axis is the disorder parameter.

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Investigations on double perovskites Pr_2MnNiO_6 and $Nd_{2-x}Sr_xMnNiO_6$: Spectroscopy and *ab-initio* studies

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The electronic structure of double perovskite Pr_2MnNiO_6 was studied using core x-ray photoelectron spectroscopy (XPS), x-ray absorption spectroscopy (XAS) and *ab-initio* calculations[1]. Based on charge transfer multiplet analysis of the Ni/Mn *2p* XPS and XAS spectra, we find charge transfer energies of 3.5 and 2.5 eV for Ni and Mn respectively. The ground state of Ni^{2+} and Mn^{4+} ions reveal a higher *d* electron count of 8.21 and 3.38 respectively as compared to the ionic values. The partial density of states show a charge transfer character of the system for $U- J \geq 2$ eV wherein an increase in *U* does not change the band gap. With increase in $U - J$, the spectral weight of O *2p* states increase below E_F, while the spectral weights of Ni and Mn *3d* states, become smaller in comparision. The O *1s* edge absorption spectra reveal a band gap of 0.9 eV, which is close to the value estimated from XPS and XAS. Our studies reveal that the material is a $p - d$ type charge transfer insulator with an intermediate covalent character as per the to the Zannen–Sawatzy–Allen phase diagram.

In second part of my talk, I shall discuss effect of Sr doping on Nd_2MnNiO_6. The compound $Nd_{2-x}Sr_xMnNiO_6$(x=0, 0.2, 0.4, 0.5 and 1) is investigated experimentally from bulk magnetization, x-ray spectroscopy and *ab-initio* methods[2]. There occurs a structural transformation from monoclinic ($P2_1/n$, for x = 0 to 0.5) to cubic ($Fm\bar{3}m$, for x = 1). The systematic reduction in magnetic moment at 5 K suggests an increase in antisite disorders with doping. Our GGA-based calculations for the ordered supercell, predict half metallic character for doping (x > 0) samples due to delocalization of Ni e_g orbitals. The theoretical magnetic moment of Mn remains constant irrespective of doping, x. However, the moment of Ni shows a drastic reduction with doping, from 1.4 μ_B to 0.7 μ_B suggesting an increase in covalent character of the system. Temperature dependent resistivity measurements exhibit a clear metallic region for x = 0.2 sample, while for x > 0.2, the metallicity gets suppressed due to increase in anti-site disorders. Calculations on supercell with anti-site disorder was systematically performed with flip of 1 and 2 Mn/Ni sites which yield drastic reduction in Ni moments. With doping, the disordered anti-ferromagnetic phase yields lowest energy, especially for x=1.

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Density of states in variational Monte Carlo

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Variational Monte Carlo is a powerful tool to study the strongly interacting electron materials with a large cluster. It is a technique that is optimized to find the ground state $|\varphi\rangle$ and to estimate average values of operator A from this ground state:

$$\langle \mathrm{A} \rangle = \frac{\langle \varphi | \mathrm{A} | \varphi \rangle}{\langle \varphi | \varphi \rangle} = \sum_{\mathrm{x}} \rho(\mathrm{x}) \frac{\langle \varphi | \mathrm{A} | \mathrm{x} \rangle}{\langle \varphi | \mathrm{x} \rangle} \qquad \text{where} \quad \rho(\mathrm{x}) = \frac{|\langle \varphi | \mathrm{x} \rangle|^2}{\langle \varphi | \varphi \rangle},$$

and $|\mathrm{x}\rangle$ is a specific state of the system. The sum over specific states is estimated using Monte Carlo sampling. In this poster, I want to show how it is possible to estimate the Green function, thus the density of state using this approach.

The Green function require the inverse of the Hamiltonian. However, for a large system, it is impossible to have a complete representation of the Hamiltonian. A solution is to approximate the Hamiltonian with a subspace composed of many different excitations and work with this new matrix in this subspace.

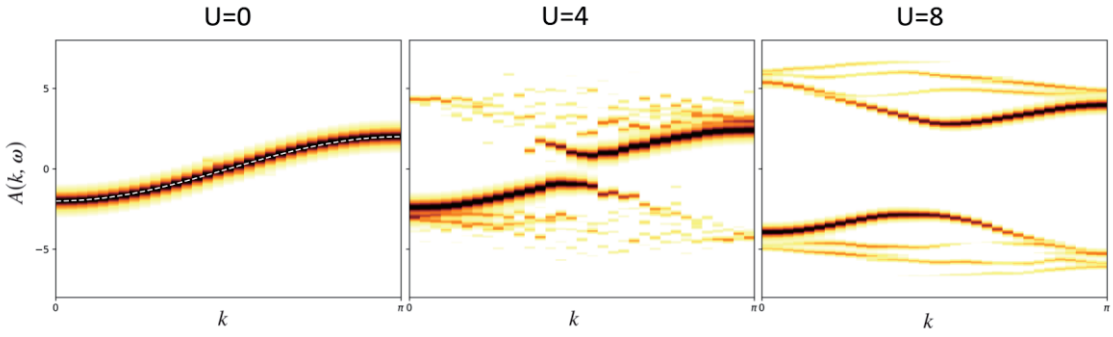

Fig. 1: Denstity of state for a Hubbard chain for different interactions levels U.

The density of state for a one-dimensional Hubbard chain is shown in Fig. 1. We can show that it correctly reproduces the Mott gap opening with interaction.

This project has been conducted with the open source package mVMC.

Reference:

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Analysis of basic properties of compact representation of many-body Green's function

Naoya Chikano, Kazuyoshi Yoshimi[A], Junya Otsuki[B], Hiroshi Shinaoka
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The Matsubara Green's function is a building block of a variety of quantum many-body theories ranging from the dynamical mean-field theory to quantum Monte Carlo methods. As the data size of the Green's function grows at low temperature, practical calculations using these methods often suffer from large computation time and massive memory consumption. Recently, some of the authors and co-workers proposed a compact representation for the imaginary-time dependence of the Green's functions [1,2,3]. The basis functions of this "intermediate representation (IR)" are a solution of an integral equation based on a physical ground. The absence of analytic and accurate numerical solutions however prevents the application of the IR to practical calculations as well as detailed analysis of its properties.

We propose an efficient numerical method for computing an accurate numerical solution of the basis functions [4]. Based on the obtained numerical solution, we study the properties of the IR basis in detail. In particular, we show that for any system the number of the required expansion coefficients grows only logarithmically with inverse temperature β (see the figure). To promote the application to the IR basis to practical calculations, we published the numerical solutions and Python/C++ libraries as "irbasis" [5]. In this presentation, we will show the result of analysis of the basic properties of the IR basis and an outline of "irbasis".

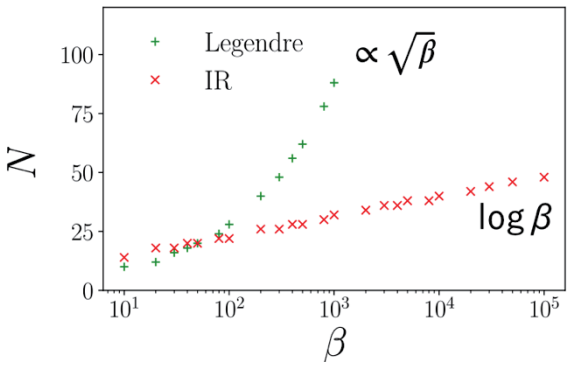

Fig.1: The number of expansion coefficients required to represent the Green's function.

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Chiral-Glass Phase in a Ceramic $YBa_2Cu_3O_7$ Superconductor at Low Magnetic Field

Hiroyuki Deguchi[1], Yuki Kato[1], Takanori Hujii[1], Masaki Mito[1], Akihiko Hisada[2], Kuniyuki Koyama[2], and Makoto Hagiwara[3]

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Ceramic cuprate superconductors composed of sub-micron size grains are considered to be made up of random Josephson-coupled networks of 0 and π junctions, and show successive phase transitions. The first transition is the intragrain superconducting one at T_{c1} and the second is the glass transition among the grains at T_{c2} ($< T_{c1}$) at which a sharp peak of nonlinear susceptibility is observed. This critical phenomenon at T_{c2} suggests the onset of the chiral-glass phase predicted by Kawamura [1]. The third transition at T_{c3} ($< T_{c2}$) is the intergrain superconducting one, where the resistivity of the ceramics becomes zero. Recently, we studied the field dependence of the intergrain transition temperatures T_{c2} and T_{c3} in the ceramic $YBa_2Cu_4O_8$, and obtained the field-temperature phase diagram of the intergrain ordering [2]. The chiral-glass phase exists in the narrow field-temperature region between the intergrain superconducting transition and the intragrain superconducting one at low magnetic field.

In this work we investigated the field dependence of T_{c2} and T_{c3} in the ceramic $YBa_2Cu_3O_7$. The field-temperature phase diagram is obtained as shown in Fig.1. The values and field dependence of T_{c3} are different from those of T_{c2} below 100 Oe. However, the transition line for T_{c2} coincides that for T_{c3} in the magnetic field above 100 Oe. The chiral-glass phase exists in the narrow region below 100 Oe. The results suggest that the chiral-glass ordering takes place at finite fields in ceramic cuprate superconductors.

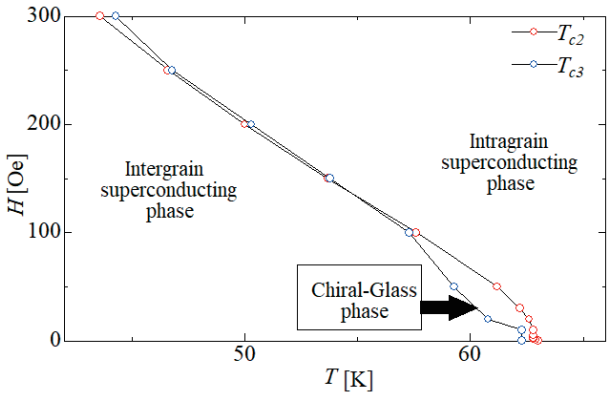

Fig. 1: Phase diagram in the ceramic $YBa_2Cu_3O_7$

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Electronic structure, chemical reactivity and optoelectronic properties of 4',5'-dibromo-2',7'-dinitro-3-oxo-3h-spiro[2-benzofuran-1,9'-xanthene]-3',6'-diolate from first principles calculations

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Abstract

In this article, the molecular structure, electric parameters and optoelectronic properties of 4',5'-dibromo-2',7'-dinitro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3',6'-diolate have been theoretically studied. We used the RHF and DFT (PBE1PBE, MPW1PW91, B3PW91 and B3LYP) approach to calculate the optimized parameters, molecular structure, electric parameters and optoelectronic properties of the tilted compound with the cc-pVDZ basis set. In addition, we calculated the chemical reactivity to show the stability of the molecule. As for the titled compound, the LUMO–HOMO energy gap value of RHF is the largest, B3LYP is the smallest, indicating the former which is slightly stable than the later. The larger the HOMO-LUMO energy gap, the harder and more stable (less reactive) the compounds. The lowest value (3.78eV) is shown in B3LYP is most stable and the highest value (8.81eV) in RHF is least stable. The energies of frontier orbitals are used to determine several chemical reactivity parameters as a measure of relative stability and reactivity. The effect of correlation decreased the value of HOMO-LUMO energy, chemical hardness and increased the

electronic chemical potential and electrophilicity. Our results suggest that this molecule have potential applications as linear and nonlinear optical materials. Due to the large hyperpolarizability of this molecule, we think that these molecules have potential applications in the field of optoelectronic and can be a promising material for optical limiting applications.

Keywords: *electronic structure; chemical reactivity; optoelectronic properties; RHF and DFT; and optical limiting applications.*

Singular *I-V* characteristics in the intermediate state of intergrain ordering of a ceramic superconductor system found by a new measuring technique

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Superconductive ceramics in which fine grains are bonded through each weak junction can show intergrain ordering as for phase angle difference between the adjacent grains. Thus, nature of the intermediate state of such weak junction network systems attracts physical interests, for it is considered to be neither normal-conductive nor super-conductive. Actually, anomaly of nonlinear resistivity has been found in the intermediate region of ceramic $YBa_2Cu_4O_8$ (Y124) in our preceding studies. However, origin of the anomaly had not been well discussed, since the intrinsic *I-V* feature was hard to be clarified. This problem is chiefly due to temperature modulation effects caused by sweeping applied current for the measurements.

Then in our work, several measurement techniques have been devised to solve this experimental problem. The basis (named SSPD) is that the pulsed applied current is used and its height is swept along sinusoidal curve across zero. Further ingenuity is that the pulse sequence is arranged alternatingly trace sine and cosine waves (named CP mode), which keeps the average electric power by the applied current constant. Utilizing these methods, intrinsic *I-V* characteristic of Y124 ceramics has been searched at the temperature region of the intermediate state of the intergrain ordering.

Figure 1 shows the *I-V* curve at 39 K revealed by SSPD and CP mode observation. We find the nonlinear nature is confined to the vicinity of the origin. The curve appears to trace dissipative region of Josephson tunneling characteristics with threshold voltage ~70 nV, though supercurrent region does not appear in the sweep cycle. Thus found nature is considered to be essential for the fluctuated intermediate state.

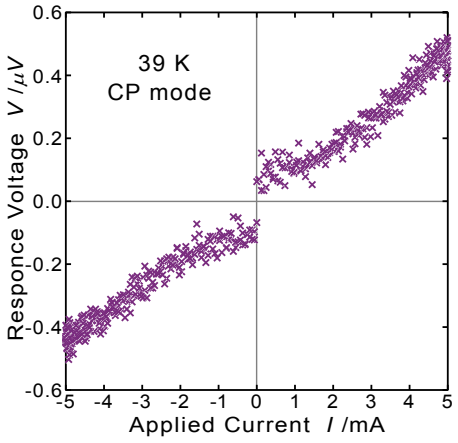

Fig. 1: Voltage (V) vs. current (I) curve for ceramic $YBa_2Cu_4O_8$ at 39 K.

Dynamical topological quantum phase transitions in nonintegrable models

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We consider sudden quenches across quantum phase transitions in the spin-1 XXZ model with single-ion-type anisotropy, where the initial state is a symmetry-protected topological phase and the ground state of the final Hamiltonian has no topological order. We demonstrate that dynamical phase transitions may occur during these quenches that are identified by nonanalyticities in the rate function for the return probability. In addition, we show that the temporal behavior of the string order parameter is intimately related to the subsequent dynamical phase transitions. Using the tools of quantum information we reveal the intrinsic entanglement structure of the time-evolved states and point out that in certain cases the dynamical quantum phase transitions are accompanied by enhanced two-site entanglement.

Study on Harmonic Response and Phonon Dispersion with Inelastic X-Ray Scattering in the Geometrically Frustrated Iridate $Ca_5Ir_3O_{12}$

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$Ca_5Ir_3O_{12}$ has a hexagonal structure with noncentrosymmetric space group of $P\bar{6}2m$ (No. 189). In the structure, 1D chains of the edge-sharing IrO_6 octahedra form triangular lattices in the *c*-plane, as shown in Fig. 1. The average valence of Ir ions in $Ca_5Ir_3O_{12}$ is +4.67, so Ir^{4+} and Ir^{5+} exist in a ratio of 1 : 2. This situation can lead to the geometrical frustration of charge on both the triangular lattice in *c*-plane and 1D chains along the *c*-axis [1]. It is reported that $Ca_5Ir_3O_{12}$ exhibits an antiferromagnetic below 7.8 K and a second-order phase transition at 105 K [1]. The origin of this phase transition at 105 K is not clear at present; this is "hidden order" [1]. Recently, nonlinear electrical conductivity along the *c*-axis in a single crystal of $Ca_5Ir_3O_{12}$ is discovered even above 105 K [2].

We performed the harmonic voltage response experiments by application of sine-wave current in order to investigate the non-linear electrical conductivity in detail. In addition, we measured the phonon dispersion by using inelastic X-ray scattering experiments at SPring-8 to reveal the origin of hidden order. We found that the phonon dispersion observed at room temperature is in good agreement with the result by GGA calculations with spin orbit interaction. We will report these results in this presentation.

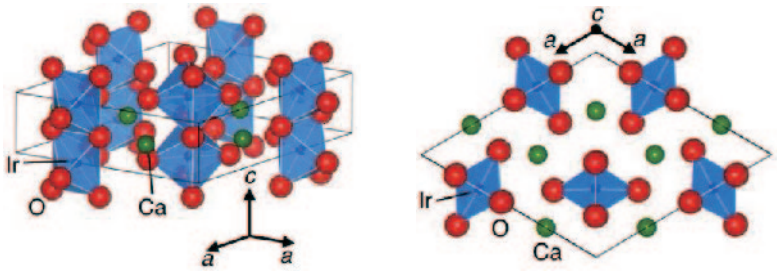

Fig. 1 Crystal structure of $Ca_5Ir_3O_{12}$ [2]

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Tensor network approach to non-equilibrium systems

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Recently, new numerical tools based on a tensor network representation is extensively developed for strongly correlated systems. Using them, we get many new results for quantum and classical phases of equilibrium systems. A tensor network represents informational correlations in a system. Therefore, it gives us a new informational point of view for a macroscopic phase of a system. However, the application of tensor network for a non-equilibrium system is not so much, and we have little understanding of the informational aspect of a macroscopic non-equilibrium system.

Here, we show new application of tensor networks for some non-equilibrium models. For example, we focus on a (1+1)-dimensional directed percolation (DP), a canonical model of a non-equilibrium continuous transition to a phase dominated by a single special state called the "absorbing" state. Using a tensor network scheme, we numerically calculate the time evolution of state probability distribution of DP. We find a universal relaxation of Renyi entropy at the absorbing phase transition point and a new singularity in the active phase where the second-order Renyi entropy has a cusp and the dynamical behavior of entanglement entropy changes from asymptotically-complete disentanglement to finite entanglement. We confirm that the absorbing state, though its occurrence is exponentially rare in the active phase, is responsible for these phenomena. This interpretation provides us with a unified understanding of time-evolution of the Renyi entropy at the critical point as well as in the active phase.

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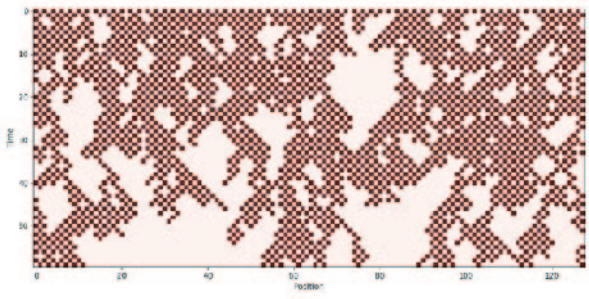

Fig. 1: The (1+1)-dimensional directed percolation at a non-equilibrium critical point.

Raman scattering investigation on geometrically frustrated iridate $Ca_5Ir_3O_{12}$

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Iridium oxides have attracted much attention as a strongly correlated electron system with strong spin-orbit interaction (SOI). The *d*-orbitals of Ir are divided into J_{eff}=3/2 and J_{eff}=1/2 states under strong SOI. $Ca_5Ir_3O_{12}$ has the intermediate valence $Ir^{14/3+}$ ions, if we assume Ca^{2+} and O^{2-} ions. The 3 J_{eff}=1/2 bands will be filled by one *5d* electron. This will lead to metallic state, which is also obtained from the *ab initio* DFT calculation [1]. However, the conductivity is insulative even at room temperature [2]. In addition, $Ca_5Ir_3O_{12}$ indicates a second order transition at T_s = 105 K; $Ca_5Ir_3O_{12}$ shows magnetic ordering at 7.8 K [2]. The transition mechanism at T_s is remains unresolved; powder X-ray and neutron diffraction experiments have not detected any structural change at T_s until now [2]. To clarify the transition mechanism at T_s, we performed Raman scattering measurements on $Ca_5Ir_3O_{12}$ [3].

$Ca_5Ir_3O_{12}$ has a hexagonal structure with noncentrosymmetric space group P-62m. The Ir-O chains along *c*-axis arrange on triangular lattice separated by Ca ions [1]. Raman active modes are $6A_1$' + 13E' + 6E''. Among them, we have observed $6A_1$' + 9E' + 5E'' at room temperature. Below T_s, new 23 peaks have been observed. This is a clear evidence of the structural change at T_s. This large number of new peaks indicates an appearance of a superlattice structure. The polarization dependence below T_s can be analyzed under -6 point group. Therefore, the -6 symmetry will conserve at the transition. Moreover, we have observed at least one new mode as a broad and weak peak from higher temperature than T_s. This suggests a possible local distortion around Ir ions above T_s, relevant to a mixed valence states of the Ir ions.

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Pressure-tuned velocity renormalization and excitonic fluctuations of 2D massless Dirac fermions in an organic conductor

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The discovery of graphene and topological materials constitutes a novel paradigm in the research of condensed matter not only for their relativistic or topological properties, but also for their potential link to the collective wisdom of strongly correlated electron systems. The 2D massless Dirac fermions in the pressurized organic conductor α-(BEDT-TTF)$_2$I$_3$ (being charge neutral due to stoichiometry) [1] provide an excellent testing ground in this regard, bringing the physics of short-range and long-range parts of the Coulomb interaction to the table; at low pressure (P) a metal-insulator transition with stripe-type charge ordering takes place in which the nearest-neighbour repulsive interaction plays a decisive role [2]. At high P, by contrast, the transition ceases above a critical value $P_C \simeq 1.0$ GPa, but instead an anomalous logarithmic increase of the Fermi velocity and excitonic fluctuations show up due to the long-rang part of the interaction [3-5] that is unscreened at the Dirac points, where the carrier density is vanishingly small.

In this talk we will report on our NMR results at a range of P in α-(BEDT-TTF)$_2$I$_3$ coupled with supportive theoretical analyses by means of renormalization-group (RG) techniques and a gap equation based on a ladder-type diagram. Focusing on the spin-lattice relaxation rate $1/T_1$ that is sensitive to the thermal excitations at the Dirac points, we show that a remarkable suppression of spin excitations develops within each Dirac cone as P is reduced towards P_C. At low temperature the additional upturn of $1/T_1$, previously reported at high P [5], shifts to a higher temperature upon decreasing P. These data are consistent with our numerical analyses signalling amplification of the log velocity renormalization and the excitonic fluctuations by the reduction of P. Probable scenarios and relevant calculations will be discussed and compared with the results.

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Effective Hamiltonian for cuprate superconductors derived from multi-scale *ab initio* scheme with level renormalization

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Mechanism of high temperature superconductivity in copper oxide superconductors discovered more than thirty years ago is still under active debates. One of the reasons of the controversies is severe competitions of completely different orders, particularly, *d*-wave superconductivity, antiferromagnetism and charge inhomogeneous states, while they are still controversial. Therefore, more quantitative *ab initio* studies are needed based on the realistic parametrization of the cuprate superconductors to reach conclusive, and quantitative understanding of the mechanism.

In this study, we propose a more accurate and realistic description of the low-energy effective Hamiltonian based on the multi-scale *ab initio* scheme for correlated electrons (MACE). We derive three-types (three-band, two-band and one-band) of effective Hamiltonians for $HgBa_2CuO_4$ and three-band effective Hamiltonian for La_2CuO_4 by improving the constrained-GW approximation combined with the self-interaction correction (cGW-SIC)[1]. The improvement for the treatment of the interband Hartree energy turns out to be crucially important, because the solution of the present improved Hamiltonian shows excellent agreement with the experimental results, for instance, for the charge gap (2 eV) and antiferromagnetic ordered moment (0.6 μ_B) of the mother compound of La_2CuO_4, in sharp contrast to the estimates by the previous Hamiltonian, 4.5 eV and 0.8 μ_B, respectively. To our knowledge, this is the first simultaneous and quantitative reproduction of these quantities by *ab initio* methods without introducing adjustable parameters. We also predict that the Mott gap and the magnetic ordered moment for $HgBa_2CuO_4$ is roughly 0.7 eV and 0.4 μ_B, respectively, if the mother compound becomes available, indicating weaker electron correlations than La_2CuO_4. The obtained Hamiltonians will serve to further clarify the electronic structures of these copper oxide superconductors and to elucidate the superconducting mechanism in an *ab initi*o fashion.

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P15

Skyrmion formation and enhanced emergent electrodynamics in centrosymmetric magnets

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*: equal contribution

Research on magnetic skyrmions, which are nanometric whirls in non-collinear magnets, has long been focused on non-centrosymmetric compounds (such as the B20 family) or interfaces, where Dzyaloshinskii-Moriya interactions favor twisted spins structures with fixed helicity.

We report on our recent experimental efforts to study skyrmion formation and associated transport responses in centrosymmetric magnets, where DM interactions are absent or cancel out globally, and where left- and right-handed spirals are nearly degenerate. In the Heisenberg systems Gd_2PdSi_3 and $Gd_3Ru_4Al_{12}$, spiral spin structures are stabilized by RKKY interactions. In applied magnetic field, a skyrmion state can be realized in these systems, as confirmed by resonant elastic x-ray scattering and real-space imaging in a transmission electron microscope. The size of a single skyrmion is typically smaller than 3 nm, resulting in a giant emergent magnetic field detectable by means of the topological Hall and Nernst effects, which have recently been observed in our laboratory.

Combining density functional theory with dynamical mean-field theory: Applications to the correlated actinide materials

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The combination of density functional theory and dynamical mean-field theory (dubbed as DFT + DMFT) is one of the most powerful and successful method that ever established to study the physical properties of strongly correlated materials. In the framework of the DFT + DMFT method, the band picture is provided by the classic density functional theory, while the electronic correlation effect is captured by a non-perturbative many-body approach, namely the dynamical mean-field theory. In this talk, I will briefly introduce the history, basic ideas, pros and cons of the DFT + DMFT method. And then I will present some selected DFT + DMFT results that my group has made in recent years about the unusual properties of some correlated actinide materials, including pressure-driven insulator-metal transition in cubic UO_2, magnetic moment puzzle in CmO_2, and valence state transition in Cf.

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Laser-controlled superconductivity in correlated electron systems

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Recently, laser-controlled superconductivity (SC) has been studied extensively to go beyond the limit of superconducting critical temperature T_c in equilibrium. An approach is a selective excitation of phonon modes of correlated electron materials by strong laser irradiation. Surprisingly, indication of superconductivity far above T_c has been observed in cuprate superconductors[1]. However, this approach is a specific one which depends on the detail of phonon modes of the material.

In this study, we propose an alternative and more general way to enhance SC in a correlated electron system without lattice degrees of freedoms. To achieve our goal, we simulated nonequilibrium dynamics in a hole-doped Hubbard model with intermediate couplings under laser irradiation by using a many-variable variational Monte Carlo method in and out of equilibrium[2,3]. For the ground states, it was shown that SC grows with increasing the on-site interaction under the charge uniform condition, but it severely competes with charge inhomogeneity in the strong coupling region [4,5].

When a charge uniform ground state is used as the initial state, we found that the SC can be enhanced by irradiating strong laser with high frequency [6]. This enhancement is caused owing to the following mechanisms. First, the effective interaction between carriers is enhanced by the dynamical localization mechanism, which drives the system into strong coupling regions. Second, the irradiation allows uniform strong SC dynamically stabilized without deteriorating into equilibrium inhomogeneities that suppress SC. We also show the results when lasers are irradiated to an inhomogeneous state. We found that the inhomogeneity dynamically melts by the same laser irradiation as that for the uniform state, and thus it causes the resultant enhancement of the SC.

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Mechanism of unconventional full-gap superconductivity in Kondo lattice with semi-metallic conduction bands

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Non-local and anisotropic Cooper pairings are usually favored in heavy-electron materials with localized *f*-electron. On the other hand, the full-gap nature of the superconducting states in $CeCu_2Si_2$ [1] and UBe_{13} [2] have been revealed by the specific heat measurements in a rotating magnetic-field. Therefore, it is desirable to propose a new mechanism of full-gap superconductivity that is specific to heavy-electron materials.

Here we theoretically study the Kondo lattice with semi-metallic conduction bands, where conduction electrons and holes compete in screening localized *f*-moment. Based on the mean-field approach, we reveal that the quantum-mechanical superposition between conduction electron and hole arises from the formation of Kondo-singlet states (Fig.1). The resultant ground state spontaneously breaks gauge symmetry to make the system superconducting. The superconducting state is characterized by the composite pair amplitude, which describes the formation of the three-body bound state composed of the conducting electron, hole and the localized spin moment [3]. We have demonstrated here that the semi-metallic conduction bands with electron and hole Fermi surfaces are closely related to the composite pairing. In addition, we discuss the possible application to real heavy-electron materials.

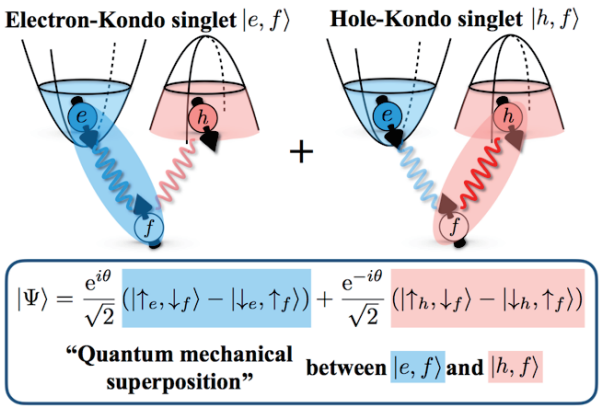

Figure 1. Conceptual picture of the mechanism of superconductivity in Kondo lattice with semi-metallic conduction bands.

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Search for excitonic condensation in $LaCoO_3$ induced at ultrahigh magnetic fields

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In a cobaltite, $LaCoO_3$, the spin-state degree of freedom of Co^{+3} (d^6) varies from high (HS), intermediate and low spin states (LS) with S = 0, 1, 2, respectively, due to the balance of Hund's coupling and crystal field splitting. A first order magnetic transition induced by magnetic field at 60 T is reported [1] from a non-magnetic ground state to a magnetized state, whose origin is still unclear. By constructing B-T phase diagram, we recently clarified that the magnetic phase is divided into two phases separated by the temperature of ~30 K [2].

Theories argue that the field induced magnetic phase may be originated in the excitonic condensation. The exotic phase appears in cobaltites as a result of the spontaneous hybridization of LS and HS states [3-5]. In excitonic condensation, the multipole order of spin and orbitals are realized the interference between different spin states, which sometimes involves nematicity of spin and orbitals.

In the present study, we have investigated the high magnetic field phase diagram of $LaCoO_3$ with magnetostriction measurements. We have developed a high speed magnetostriction measurement system for detecting the spin-state evolution of $LaCoO_3$ [6]. So far, we have confirmed that the B-T phase diagram of $LaCoO_3$ constructed by the magnetization measurement is complemented by the magnetostriction measurement.

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Development of Orbital-Free Density Functional Theory with Machine Learning

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Orbital-free density functional theory (OFDFT) circumvents the use of N single-particle orbitals for the expression of the non-interacting kinetic energy functional, where N is the number of electrons in the system. The explicit formulation of the kinetic energy term makes it possible to simulate systems that consists of more than 10^5 atoms with the computational cost of $O(N)$. However, such an explicit formula with desired accuracy, especially in non-metallic systems, has been a long-standing question.

In this work, we construct a semi-local kinetic energy density functional (KEDF) for semiconductors via the multilayer neural network (NN), which is widely used in the context of supervised machine learning. We adopt the electron density and its gradients up to the second order as the descriptor for the NN, whereas the kinetic energy density is taken as the response variable. The training data has been adopted from diamond Si and diamond C. After the training, we have found that the NN KEDF that depends on up to the second-order density gradient can approximate the kinetic energy density better than any conventional KEDFs in diamond Si, diamond C, and zincblende SiC.

We also perform OFDFT electron density optimization using the NN KEDF and its functional derivative. We have developed a real-space OFDFT (RS-OFDFT) code, which is an MPI- and OpenMP-paralleled real-space finite-difference code. The structural properties obtained by the NN KEDF have shown fairly good agreement with the experimental values in the case of diamond Si, diamond C, and zincblende SiC. However, the convergence of OFDFT density optimization is extremely slow, especially when the NN KEDF is employed. We will present several algorithms to solve such a convergence problem along with numerical results obtained by implementing the new optimization algorithms in the RS-OFDFT code.

Optical rectification of spin current in magnetic insulators

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Insulator spintronics has considerable advantages over the metallic counterpart. Spin current in the insulators are carried by chargeless magnetic excitations; it is decoupled from charge current and free from Ohmic loss. In addition, the relaxation time of angular momentum is typically longer in the magnetic insulators. Owing to these potential advantages, insulator spintronics has become an active field in the spintronics.

Despite the increasing interest, the method of generating spin current, especially, with electromagnetic waves has been less explored. Unlike the electronic excitations, the chargeless magnetic excitations do not couple to scalar potential. Therefore, the control of spin current by the electromagnetic fields is generally difficult. In this talk, we propose a novel method for generating spin current using nonlinear optical effects. Using a nonlinear response theory, we study the generation of spin current in antiferromagnets. We show that the three types of spin-light couplings induce a dc spin current in a spin chain with a spin-liquid ground state: inverse Dzyaloshinskii-Moriya, Zeeman, and magneto-striction couplings [1]. We find that the dc spin current appears in a model in which the total spin angular momentum is conserved. This is in sharp contrast to the established methods such as spin pumping in insulators and optical spin-current generation in metals. Our results also imply that the spin-orbit interaction is unnecessary for the generation of spin current [2]. This is a potential advantage for application because the spin-orbit interaction tends to shorten the relaxation time of spin angular momentum.

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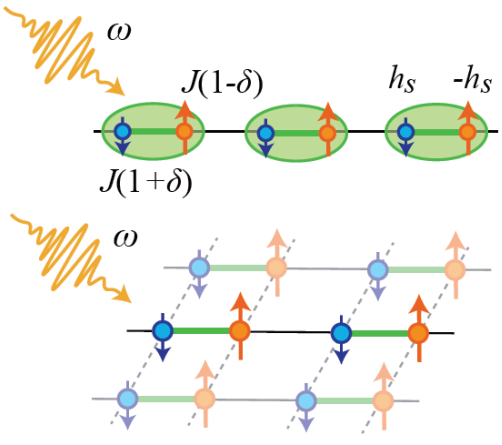

Fig. 1: Schematic figure of the noncentrosymmetric magnets we considered. A linearly-polarized THz light is applied to the magnetic insulator to generate spin current.

Nature of superconducting fluctuation in photo-excited systems

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By using pump-probe spectroscopy, the light-induced superconductivity (SC) have been proposed in 2D systems such as $La_{1.675}Eu_{0.2}Sr_{0.125}CuO_4$ [1] or $YBa_2Cu_3O_{6.45}$ [2] above the transition temperature. Also in the 3D material, K_3C_{60}, whose SC transition temperature is T_c=19.8K, it is suggested that light-induced SC can arise at around 100K [3]. These experiments have attracted much attention recent years. As for the theoretical researches, it is discussed that the induced photons cause the change in the effective interaction among electrons through the change in phonons by lights, and also the direct effect to the electronic systems and so on [4-7].

In this study, we study the superconducting fluctuation effects in photo-excited systems above the transition temperature. We have analyzed the pump-probe spectroscopy theoretically by using time dependent Ginzburg-Landau theory with a simple setup shown in Fig.1. The SC fluctuation and current, which is induced from pump-lights, show exponential decay in long-time limit. For a short-time behavior, by contrast, we have revealed that they behave in a non-trivial manner: power-law and logarithmic decays are found depending on the spatial dimensions. The non-equilibrium component of the current, which derives from probe-lights has always negative contribution after injecting the lights in each spatial dimension. In this poster presentation, we will discuss the change of the SC fluctuation, current and paraconductivity as functions of evolving time and pump-light amplitude.

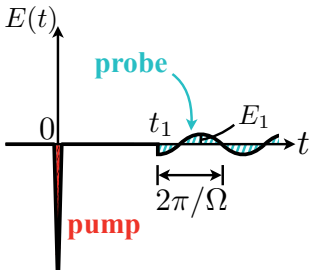

Fig. 1: A sketch for the model of the electric field considered in our theory. E_1 and Ω means the intensity of the electric field and its frequency of the probe-lights.

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Chromium breathing pyrochlores as a showcase for a variety of pyrochlore Hamiltonians

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We investigate all six structurally characterized chromium-based breathing pyrochlores using a combination of density functional theory and pseudofermion functional renormalization group calculations. We show that the distinct magnetic behavior of the materials $LiInCr_4O_8$, $LiGaCr_4O_8$, $LiInCr_4S_8$, $LiGaCr_4S_8$, $CuInCr_4S_8$ and $CuInCr_4Se_8$ can be matched one-to-one to their chemical composition, namely, oxides, sulfides and the selenide, with each realizing very different pyrochlore Hamiltonians. While the oxides form breathing pyrochlore antiferromagnets displaying correlations reminiscent of a perturbed Coulomb spin ice phase, in the sulfides, the ground state degeneracy exhibits a dimensional reduction leading to line-like degeneracies in momentum space originating from an effective face centered cubic lattice mapping in the low temperature regime. In the selenide we reveal the presence of an approximate spiral spin liquid characterized by a sphere-like degenerate manifold of states in reciprocal space. This rich variety of effects is rooted in the subtle interplay of longer-range exchange couplings, up to third nearest-neighbor on the pyrochlore lattice, and also holds the key to successfully describing the available experimentally observed magnetic response of the sulfides and the selenide.

Metallic Spin Liquid-like Behavior of LiV_2O_4

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Quantum phase transition and associated critical behavior of electronic states has been a central focus of condensed matter physics in the past decades. In particular, the "metallic spin-liquid" state is attracting much interest as a novel non-Fermi liquid state, where it is predicted to emerge near the quantum critical point (QCP) next to the spin-glass state. Furthermore, the metallic spin liquid is intensively discussed as a stage for application of the so-called anti-de-Sitter/conformal field theory (AdS/CFT) correspondence developed in the quantum field theory of gravity and entropy of black holes.

In this contribution, we suggest that LiV_2O_4 spinel would serve as a promising stage for the understanding the metallic spin liquid [1]. LiV_2O_4 is known to exhibit heavy fermion-like behavior below a characteristic temperature T_K~20 K, while it preserves a paramagnetic state down to ~10^{-2} K due to geometrical frustration. We show that the dynamical spin susceptibility $\chi(\mathbf{q},\omega)$ in LiV_2O_4 exhibits anomalous duality which is modeled as a sum of itinerant (χ_F) and local (χ_L) components, and that the behavior of $\chi_L(\mathbf{q},\omega)$ inferred from muon experiment is in line with that theoretically predicted for the metallic spin liquid [2]. The anomaly coexists with the marginal Fermi-liquid behavior inferred from the $-\ln T$ dependence of the electronic specific heat over a wide temperature range below T_K. We argue that such unusual properties of LiV_2O_4 can be attributed to the putative metallic spin liquid state emerging near QCP between spin glass and Fermi liquid states.

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Tensor network approach to the Kitaev spin liquid

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The Kitaev spin liquid has attracted much attention because of its exact solvability [1] and possible realization in Iridium and ruthenium compounds [2]. However, the effective models may include additional spin exchange interactions that could destabilize the spin liquid [3]. General-purpose numerical methods that do not resort to the Majorana fermion representation are needed for solving such generalized models.

To this end, we investigate the applicability of the two-dimensional tensor-network method in the Kitaev honeycomb systems. We first demonstrate the usefulness of the tensor product state (TPS) or the projected entangled-pair state (PEPS), which is described in the spin degrees of freedom, in the simplest isotropic ferromagnetic Kitaev model. We construct an optimal TPS in a small bond dimension (D=2) according to the required physical symmetries as well as the vortex-free configuration of the $\mathbf{Z}_2$ gauge field. This ansatz state already exhibits the criticality of the exact Kitaev spin liquid [4]. In contrast to the previous study [5], the lower-cost imaginary time evolution (simple update) is found to be enough to obtain accurate energy for D=4. The energy is further improved as D is increased.

We then make use of this ansatz for more generalized Kitaev models that contain the interaction anisotropy, the Heisenberg exchange interaction, and the magnetic field. For all cases, we find the presence of the Kitaev spin liquid *phase*.

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Liquid dynamics of orbital molecules with long correlation length in layered $LiVS_2$

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Electronic instabilities in transition metal compounds often lead to the complex arrangement of orbital molecules in a spin singlet state in low temperature. Examples include dimer in Li_2RuO_3 [1] and pairs of trimer and tetramer in AlV_2O_4 [2]. Recent local structural studies utilizing the pair distribution function (PDF) revealed that the disordered orbital molecules appear ubiquitously even in high temperature paramagnetic phases [3]. The central issue to be solved is whether such disordered orbital molecules exhibit liquid-like dynamics or glass-like statics.

To address this issue, we performed the structural studies of $LiVO_2$ and $LiVS_2$ with triangular lattices. Although high temperature metallic nature in $LiVS_2$ is significantly different from the insulating behavior in $LiVO_2$, both compounds enter the nonmagnetic insulator state in low temperatures [4]. In $LiVO_2$, the low temperature orbital molecule patterns were conjectured to be trimer by J.B. Goodenough on 1963 [5], although it has never been crystallographically clarified. Meanwhile, low temperature orbital molecule patterns remain unclear in $LiVS_2$.

Here, we present that vanadium trimers are crystallographically clarified both in $LiVO_2$ and $LiVS_2$ in low temperature phases. Remarkably, upon heating higher than the trimer transition temperature of 314 K in $LiVS_2$, the trimer molecules completely disappear and, instead, disordered zigzag chain molecules with long correlation length of several hundred angstrom appear with fluctuating in the order of msec~sec.

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Quantum Critical Phenomena in Heat Transport via a Qubit

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Quantum critical phenomena (QCP) near zero-temperature second-order phase transition have been studied for long time in condensed matter physics. It is still challenging to realize them in controlled experimental systems, and has recently been studied, e.g., via transport properties in multi-channel Kondo quantum dots [1]. In this presentation, we consider heat transport carried by photons via a quantum two-state system (a qubit) [2]. For an appropriate environment (the sub-ohmic reservoir), it is known that the system undergoes quantum phase transition at a critical system-reservoir coupling. We discuss QCP in heat transport through temperature dependence of a thermal conductance [3]. We also propose a superconducting circuit coupled to a flux qubit as a feasible experimental system realizing the sub-ohmic reservoir. We expect that recent development in calorimetry will enable us to observe QCP proposed here in near future. This work is the collaborated research with Tsuyoshi Yamamoto.

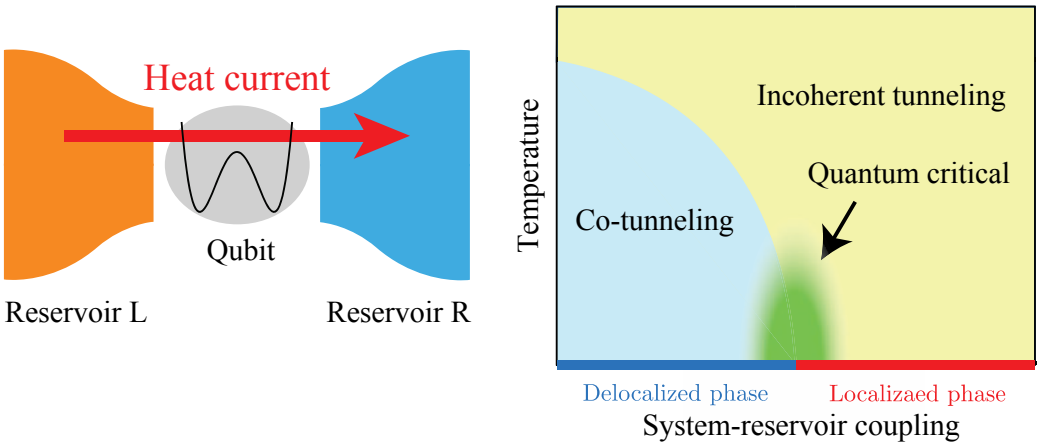

Fig. 1: (Left) A schematic of heat transport via a qubit. (Right) The phase diagram of the qubit coupled to the sub-ohmic system.

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Poster Presentations – Section B

Microscopic Investigation of a phase transition between an insulator $CaCu_3Ti_4O_{12}$ and a metal $CaCu_3Ru_4O_{12}$: Cu-NQR in $CaCu_3Ti_{4-x}Ru_xO_{12}$

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A-site-ordered cubic perovskite systems, $CaCu_3B_4O_{12}$, are regarded as perovskite systems ABO_3 involving periodically-ordered nonmagnetic Ca and Jahn-Teller Cu ions at A site. For the B = Ti case, $CaCu_3Ti_4O_{12}$ is an antiferromagnetic insulator showing an enormously large dielectric constant [1], although a Ru member, $CaCu_3Ru_4O_{12}$, is a paramagnetic metal [2,3,4]. The 3*d* electron at Cu changes its nature from an insulating state to an itinerant. In fact, the complete solid solution system, $CaCu_3Ti_{4-x}Ru_xO_{12}$ (CCTRO), which was first synthesized using a high-pressure technique and its macroscopic properties were measured by our group, shows an insulator-to-metal transition with the Ru content x [5]. A Mott transition picture was safely applied, where a critical line of the two phases is considered to appear around $x_c \sim$ 2-3 [5].

We perform a Cu-NQR study on CCTRO, in order to investigate microscopic change of the Cu-3d electron through the transition. The ^{63}Cu spectrum in CCTRO consists of seven peaks with their central frequencies unchanged along x. This could be understood in terms of Cu-site-splitting arising from local coordination of the neighboring B site ions (Ti/Ru), which also implies the used samples are chemically homogeneous. For a sample with $x > 2.0$, $1/T_1T$ of each peak are similar in value at high temperatures and shows a temperature independent behavior, indicating existence of a metallic phase in the sample. The $1/T_1T$ value at high temperatures is larger as x decreases. This corresponds to an increase of the density of the state at Fermi surface toward the transition to an insulating phase, which might coincide with the Mott transition picture. Moreover, around x_c, significant temperature dependence of $1/T_1T$ is seen below ~ 100K, where the magnitude varies with the measured peak. The origin is discussed in terms of microscopic coexistence of the metallic and insulating phases.

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Topological classification of non-Hermitian insulators and superconductors

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Non-Hermiticity [1,2] enriches topological phases beyond the existing framework for Hermitian topological phases. Whereas unusual features with no Hermitian counterparts were extensively explored [3-5], a full understanding about the role of symmetry and topology in non-Hermitian physics has still been elusive. In particular, complete topological classification of non-Hermitian insulators and superconductors has yet to be established, which serves as a non-Hermitian generalization of the 10-fold classification of Hermitian ones [6,7] according to the Altland-Zirnbauer internal symmetry [8].

Here we develop a general classification theory of non-Hermitian topological phases [9]. We demonstrate that non-Hermiticity ramifies the celebrated Altland-Zirnbauer symmetry classification for insulators and superconductor, leading to 38-fold symmetry class instead of the 10-fold one. Moreover, we reveal that two types of energy gaps are relevant for non-Hermitian systems due to the complex nature of energy spectra. Based on the 38-fold symmetry and the two types of complex-energy gaps, we complete classification of non-Hermitian topological phases in arbitrary dimensions and symmetry classes. Our work establishes a theoretical framework for the fundamental and comprehensive understanding of non-Hermitian topological phases and paves the way towards uncovering unique phenomena and functionalities that emerge from the interplay of non-Hermiticity and topology.

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Spin and charge correlations across the extended pseudogap regime in the half-filled 2d Hubbard model

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The Hubbard model at half-filling on the square lattice is known to feature a crossover from metal to antiferromagnetic (AF) insulator via the extended pseudogap regime. We study spin and charge correlation functions across the pseudogap regime with controlled accuracy using the diagrammatic Monte Carlo approach and provide reliable benchmarks for experimental verification with quantum emulators on optical lattices in the currently accessible temperature range. The charge and spin correlation functions change their character as the system crosses over from metal to AF insulator. Near the AF insulator regime, we observe the strongly enhanced AF peak in spin correlation and overall suppressed charge correlations. The charge correlation function, however, changes its temperature dependence at sizably weaker interaction strength compared to the spin correlation function. In terms of the energetics, we show that there exists the subregion within the extended pseudogap regime, where the system gains both the kinetic and potential energy simultaneously as the temperature decreases.

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Electronic States in Organic Conductor α-$(BETS)_2I_3$

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The two dimensional electron system in the organic conductor α-$(BEDT\text{-}TTF)_2I_3$ has attracted much attention, since it exhibits a unique metal-insulator transition at T=135K. The metal and insulator phases have been attributed to the massless Dirac electron phase with the inversion symmetry and charge order phase due to the inversion symmetry breaking, respectively [1-3].

The organic conductor α-$(BETS)_2I_3$, being a related material of α-$(BEDT\text{-}TTF)_2I_3$, exhibits the characteristic transport and NMR properties similar to the Dirac electron phase in α-$(BEDT\text{-}TTF)_2I_3$ at T>50K [4,5]. The low temperature phase at T<50K is an insulator, while the phase transition is unclear. In contrast to α-$(BEDT\text{-}TTF)_2I_3$, however, the inversion symmetry is not broken in the low temperature phase.

The numerical results of the extended Hückel method [6] and the 1st principle calculation [7] indicates that α-$(BETS)_2I_3$ is a semimetal with both electron and hole pockets. As a candidate of the low temperature phase, a band insulator induced by the mean field of the nearest neighbor Coulomb interactions has been proposed [8]. It is also proposed that the spin-orbit interaction play an important role [9]. Thus the electronic state of α-$(BETS)_2I_3$ is still controversial.

In the present study, an extended Hubbard model describing α-$(BETS)_2I_3$ is derived using the 1st principle calculation. The electronic state is examined using the mean field theory and the exact diagonalization.

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Coupled Spin-Charge Fluctuation in the Semimetal Phase of All-In/All-Out Antiferromagnet $Cd_2Os_2O_7$

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We report on a novel electromagnetic f uctuation in $Cd_2Os_2O_7$ pyrochlore over the temperature range where the all-in/all-out (AIAO) antiferromagnetic order below $T_N \simeq 227$ K coexists with the semimetal phase above $T^* \simeq 150$ K. Muon depolarization observed for $T^* < T < T_N$ indicates that the magnetic f uctuation is induced by the metallic carriers conducting on the AIAO spin texture. Remarkably, the relevant spin-charge dynamics is hidden to other magnetic probes, suggesting local character of excitation associated with strong spin-orbit coupling and a peculiar frequency range of f uctuation ($\sim 10^7$–10^{10} s^{-1}) uniquely accessible to muon. The onset of such a coupled spin-charge excitation is presumed to enhance electric resistivity to mimic metal-insulator (MI) transition at T_N, while the true MI transition occurs around T^* upon opening of the indirect charge gap. We also discuss possibility for the formation of a magnetic polaron-like band in the semimetal phase.

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Correlated higher-order topological insulator on kagome lattice

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The electron-electron correlation gives birth to a variety of nontrivial topological phenomena. One of the typical examples is the topological Mott insulator [1,2] hosting gapless edge spin excitations. Its difference from the conventional topological insulators (TIs) is the absence of the gapless charge excitations at the edge, which is driven by the strong correlation effects. Two-dimensional higher-order TIs [3], which support gapless topological corner states although edge states are gapped, are a new class of topological phases. While it is expected that the electron-electron interactions also bring further diversity to higher-order TIs, the theoretical studies for correlated higher-order TIs are sparse.

In this poster, the correlation effects on the higher-order TIs are investigated by solving the kagome Hubbard model exhibiting the corner states in the noninteracting case [4] [see Fig. 1 (a)]. We numerically demonstrate that the electron-electron correlation results in the gapless corner spin excitations. Figure 1 (b) shows the energy spectrum given by the effective spin Hamiltonian for the open system as a function of $\tan\phi = t_B/t_R$, where t_B (t_R) is the nearest-neighbor hopping parameter associated with the upward (downward) facing triangles. The result indicates that the ground state is accompanied by the 8-fold degeneracy for $0 \leq \phi \lesssim \pi/4$, which suggests the presence of the higher-order corner states where the spin excitation is gapless. We also confirm that the spin counterpart of the Z_3 Berry phase [5], the topological invariant detecting the upward or downward trimers pattern, characterizes the correlated corner-Mott states.

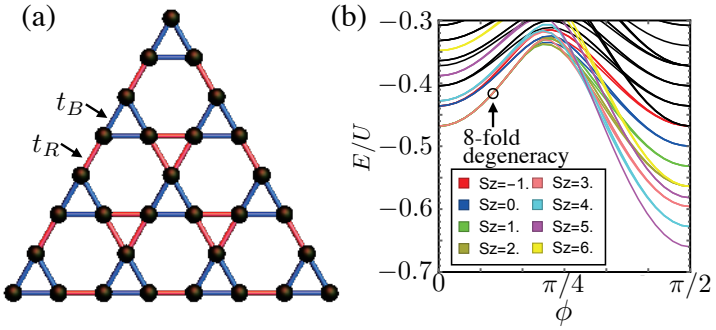

Fig.1 (a) Sketch of kagome lattice and the boundary condition. (b) Energy spectrum E/U as function of ϕ. U is the strength of the interaction. The total S_z is expressed by the color of plots.

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Supercurrent generation by spin-twisting itinerant motion of electrons in a model for cuprate superconductors

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Superconductivity is a phenomenon in which externally supplied electric current flows through a system without voltage drop. This current flowing state is dissipationless, thus, thermodynamically stable. At zero temperature, this will lead to the conclusion that this current flowing state is energetically stable one, thus, must be one of local energy minimum states.

In the BCS theory based understanding, the mechanism for the supercurrent generation is explained using the dc Josephson effect. The Josephson effect occurs in a superconductor-insulator-superconductor junction (Josephson junction), where the insulator part is so thin that electrons can tunnel through it. Josephson considered the Cooper pair tunneling through it; each superconductor in the junction is assumed to be characterized by the phase conjugate to the Cooper pair number and predicted that the dissipationless current is generated by the difference of the phases of the two superconductors. Then, regarding superconductor as a collection of Josephson junctions, the supercurrent in a superconductor is explained as due to the gradient of the phase. However, this explanation does not guarantee the existence of an energy minimum under the external current feeding condition.

Through the study of high temperature superconductivity in cuprates, a new supercurrent generation mechanism has been proposed by one of the present authors. The spin-twisting circular motion of electrons is shown to generate supercurrent. In the present work, we further consider this mechanism. We will show that if the Rashba spin-orbit interaction exists, energy minima occur at nonzero feeding current [1]. We have found such minima in the system exhibiting spin twisting itinerant motion. The supercurrent is shown to have the London equation form that exhibits the flux quantum h/2e.

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Electron Correlation in the Anomalous Muonium in Silicon

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The muon spin resonance (μSR) is an effective tool to determine the dynamics of hydrogen in materials [1,2]. The most stable atomic configuration of muonium in silicon is located at the bond center and is commonly recognized as anomalous muonium [3,4]. Several first-principles calculations have already been done but the origin of the negative Fermi contact interaction constant (FCIC) has not been clarified [5-7]. In this study, we carry out reliable first-principles calculations and quantitatively reproduce the experimental FCIC [4]. We find that a large size of supercell is necessary to obtain reliable results. Furthermore, by analyzing calculation results, we clarify that the negative FCIC is due to the electron correlation effect, i.e., we find that the negative value is not explained based on a simple one-electron approximation which leads to the zero value and the electron correlation effect induces the negative value.

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Magnetic-field-induced insulator-metal transition in W-doped VO_2

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VO_2 undergoes a first-order metal-insulator (MI) transition at 340 K [1] along with dimerization of vanadium atoms. Although the MI transition has been studied for more than 60 years, the mechanism of the transition is still highly controversial [2-4]. It has been claimed that the electron-electron correlation is fundamentally important, and thus VO_2 is a Mott-Hubbard insulator [2] or a Peierls-Mott insulator [3]. On the other hand, there is an another aspect that the structural instability of VO_2 is essential and formation of a molecular orbital of the V-V dimer causes the localization of the *d* electrons, resulting in the MI transition [4].

In the present work, we have investigated the near-infrared optical-transmission in a $V_{1-x}W_xO_2$ (x = 0.06) thin film [5] at ultrahigh magnetic fields of up to 520 T and 14 K. The MI transition temperature of the x = 0.06 film is around 86 K which is lower than that of pure VO_2 [6]. The magnetic field is generated by the electromagnetic flux compression technique [7]. The wavelength of a laser line used is 1.977 μm.

A distinct field-induced decrease of the transmission was observed at fields greater than 120 T and the transmission becomes as weak as that in the room-temperature metallic phase at 490 T, which indicates that the magnetic-field-induced insulator to metal transition occurs. Since origins of the MI transitions in VO_2 and $V_{1-x}W_xO_2$ (x = 0.06) are essentially the same [6], the observed field-induced metallization suggests the collapse of the V-V dimers; the molecular orbital of the pair of V^{4+} (d^1, s = 1/2) ions would be suppressed by magnetic field when the spin singlet state becomes unstable.

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Doping a rare-earth permanent magnet: *ab initio* studies on the impacts in multiple energy scales

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Rare-earth permanent magnet (REPM) poses us important problems both technologically and fundamentally. A practical question concerns the prospect for exploiting a bunch of good magnetic properties in the typical operation temperature range spanning from T_L=300K to T_H=450K on the basis of *4f-3d* intermetallic ferromagnets without too much of rare metals [1]. Prerequisites include a) strong magnetization, b) accordingly strong Ising-type anisotropy, c) Curie temperature that is high enough compared to T_H, all of which backed-up by d) robust crystal structure. Gaining all of these is rare: Nd-Fe-B magnet made of the particular champion magnet compound $Nd_2Fe_{14}B$ [2] has been excellent except for its relatively low Curie temperature at 585K. Here a trade-off goes on between the strong magnetization and the Curie temperature. A possibility to go beyond $Nd_2Fe_{14}B$ was suggested by *ab initio* prediction for $NdFe_{12}N$ and subsequent fabrication of a thick-film sample on a special substrate [3]. Here the structure stability is traded off by the other three properties. These competing trends span multiple characteristic energy scales. That is, a) comes from the energy scale of O(1) eV in the exchange splitting of *3d*-electron bands in Fe-based part, b) amounts to 1meV - 10meV at most c) is the order of 0.1 eV, and formation energy associated with d) comes slightly below 100 meV per atom for $Nd_2Fe_{14}B$. While celebrated Slater-Pauling curve can in principle be a guideline to maximize the magnetization with an optimal Fe-Co mixing ratio, the above competing energies in multiple-scale hierarchy and a particular lattice expansion in REPM complicates the problem. We discuss the possible improvement of REPM compounds by inspecting the effects of various elements doped into $Nd_2Fe_{14}B$ from first principles by combining structure optimization and coherent potential approximation [4]. A marginal space between $Nd_2Fe_{14}B$ and a possible maximum in the intrinsic magnetic properties is identified, in which $NdFe_{12}N$ seems to be located.

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Low-energy effective models of spin-*S* anisotropic Kitaev models

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It is known that the *S*=1/2 Kitaev model has a quantum-spin-liquid ground state with topological order as an exact solution [1]. In an anisotropic limit, it is mapped to the toric code [2], which is a promising application to the topological quantum computation. Recently, the extension to arbitrary spin for the Kitaev model has been done to understand the Kitaev model from the theoretical viewpoint [3-7].

In this presentation, we clarify low-energy properties of spin-*S* Kitaev models in an anisotropic limit. First, we derive the low-energy effective form of the local conserved quantity [3], which is found out to be explicitly different between the half-integer spin and integer spin cases. Next, we show the low-energy effective Hamiltonian, which is obtained by the simple perturbation theory. As expected by the effective form of the local conserved quantity, the form of the effective Hamiltonian is also different between the half-integer spin and integer spin cases. In the former case, the effective model is mapped to the toric code as well as the case of *S*=1/2, whose ground-state degeneracy depends on the topology of the surface. On the other hand, in the latter case, the effective model is equivalent to a free spin model under a uniform magnetic field, whose ground state is nondegenerate [8].

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Theoretical Study on the Magnetism-Driven Negative Thermal Expansion Phenomenon in the Inverse-Perovskite Antiferromagnets

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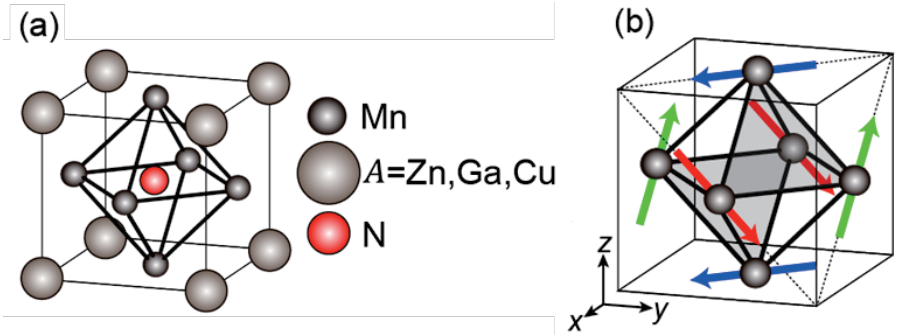
We will discuss our recent theoretical studies [1,2] on the magnetism-driven negative thermal expansion (NTE) phenomenon in the inverse perovskite antiferromagnets Mn_3AN (*A*=Zn, Ga, etc.). It was experimentally discovered almost 50 years ago that the NTE occurs in Mn_3AN triggered by a magnetic phase transition, where the crystal volume expands abruptly as the system enters a specific non-coplanar antiferromagnetic phase called Γ^{5g}-type upon cooling. Because composites of usual and NTE materials enable us to realize the zero-thermal-expansion materials, social demands on NTE materials rapidly increase along with the development of nanotechnology and precision optical and mechanical devices, in which slight changes in length and volume become fatal.

In this study, we theoretically investigate a mechanism and properties of the NTE phenomenon in Mn_3AN based on a classical spin model with competing bond-length-dependent spin-exchange interactions. We numerically reproduced the experimentally observed volume expansion upon cooling triggered by the Γ^{5g}-type antiferromagnetic order and revealed that the expansion occurs so as to maximize an energy gain of the nearest-neighbor antiferromagnetic interactions. The mechanism revealed is found to be not specific to the inverse perovskite magnets but might be expected also in magnets with other crystal structures.



(a) Inverse-perovskite type structure of Mn_3AN, (b) Γ^{5g}-type antiferromagnetic order.

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Ground-state phase diagram of the Kitaev-Heisenberg model on a kagome lattice

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The Kitaev-Heisenberg model on the honeycomb lattice has been studied for the purpose of finding exotic states such as quantum spin liquid and topological orders. On the kagome lattice, in spite of a spin-liquid ground state in the Heisenberg model, the stability of the spin-liquid state has hardly been studied in the presence of the Kitaev interaction. Therefore, we investigate the ground state of the classical and quantum spin systems of the kagome Kitaev-Heisenberg model. In the classical system, we obtain an exact phase diagram that has an eight-fold degenerated canted ferromagnetic phase and a subextensive degenerated Kitaev antiferromagnetic phase. In the quantum system, using the Lanczos-type exact diagnalization and cluster mean-field methods, we obtain two quantum spin-liquid phases, an eight-fold degenerated canted ferromagnetic phase similar to the classical spin system, and an eight-fold degenerated **q=0**, 120^{o} ordered phase induced by quantum fluctuation.

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DSQSS – PIMC solver for quantum lattice model

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The path-integral Monte Carlo method (PIMC) is one of the most powerful numerical methods for studying quantum many-body problems [1]. By using PIMC we can calculate the expectation value of an observable within a statistical error even for very large systems in arbitrary dimension at finite temperature as long as the system is free from the sign problem. The Monte Carlo method generally suffers from the slow convergence near the critical point (critical slowing down). For discrete space problems, several update methods, e.g. the loop algorithm and the directed-loop algorithm, have been developed to overcome the critical slowing down. These methods have been extended for massive parallelization for modern supercomputers [2,3].

We are developing a PIMC program package for quantum lattice problems, which we call DSQSS (Discrete Space Quantum Systems Solver) [4]. Since DSQSS adopts the directed-loop algorithm for update scheme, it can update configurations effectively even under a symmetry-breaking field, such as magnetic field and chemical potential. By editing two XML files, a lattice XML file describing how bonds connect sites and an algorithm XML file describing how worm heads should be scattered at vertices, users can perform calculation for any model on any lattice (graph). Since these XML files are complicated, DSQSS comes with utility tools to generate these files for commonly-studied models and lattices such as XXZ spin models and hypercubic lattices. DSQSS also offers the parallelized multi worm algorithm for massively parallel calculation[3]. DSQSS v2, the latest stable version, came in March 2019 with several new features such as more user-friendly interfaces. In the presentation, we will introduce DSQSS, explain the basic usage, and show some calculation results.

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Real-space observation of electronic crystallization

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Electron-electron Coulomb interactions are frustrated in the quasi-2D organic conductors, θ-(BEDT-TTF)$_2$RbZn(SCN)$_4$, in which holes in a quarter-filled band are interacting on an anisotropic triangular lattice. This material exhibits a charge ordering at ~200 K whereas rapid cooling (faster than ~ 5 K/min) suppresses the charge ordering, which gives way to supercooled liquid or glassy freezing [1,2]. The previous resistance and NMR measurements suggested that the supercooled charge liquid and glass evolves into the charge order (electronic crystallization) through nucleation and subsequent growth, which have been widely observed in atomic and molecular systems [3,4].

We have examined the spatial profile of the electronic crystal growth in this system by Raman imaging, exploiting the distinct Raman spectra in the charge-ordered and charge-glass (or supercooled) states (Fig.1). Just below the charge-order temperature, the supercooled liquid evolves rapidly and inhomogeneously into the charge order once a nucleation occurs after a long incubation time, whereas the crystallization from the glass at low temperatures evolves slowly in the form of finely distributed microcrystals (Fig.1). This behavior is consistent with the well-known nucleation and growth mechanism.

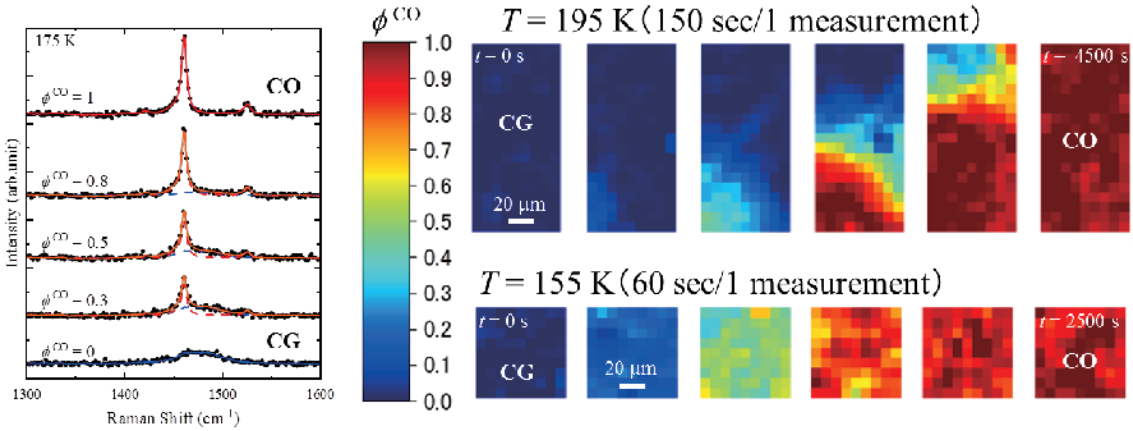

Fig. 1:(left) Raman spectrum of the *MM*' = RbZn salt. (right) The crystallization at high temperature (up) and at low temperature (down).

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Organic antiferromagnet as a spin current generator

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Spin current–a flow of electron spins without a charge current–is an ideal information carrier free from Joule heating for electronic devices. The spin Hall effect [1,2], which arises from the relativistic spin-orbit coupling, enables us to generate and detect spin currents in inorganic materials, taking advantage of their constituent heavy atoms. In contrast, organic materials consisting of molecules with light elements have been believed to be unsuited for spin current generation. Here we show that a class of organic antiferromagnets with checker-plate type molecular arrangements, such as a typical strongly correlated system κ-(BEDT-TTF)$_2X$ [3], can serve as a spin current generator. The mechanism relies on a peculiar spin splitting of the energy bands and a real space anisotropy of the electron transfers, owing to the pattern of molecular orientation and antiferromagnetic ordering. Reanalyzing the well-studied Hubbard-type model [4], we show that a spin current can be generated by applying a temperature gradient in the antiferromagnetic insulating state or an electric field in the doped metallic state [5]. We find that the spin-current conductivity is given by a symmetric tensor, in stark contrast to the spin Hall or spin Nernst effect described by an antisymmetric tensor. Our findings provide another route to create a spin current and open a new field of spintronics based on organic magnets having advantages of small spin scattering and long lifetime.

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Non-equilibrium dynamics of fractional excitations in Kitaev spin liquids

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Insulating magnets provide a good playground for quantum many-body effects on the spin degree of freedom of electrons in solids. Among them, quantum spin liquids (QSLs), where any magnetic orders are absent even at zero temperature, have attracted great interest for a number of decades as it could exhibit topological orders and possess fractional excitations with unconventional statistics. Particularly, the Kitaev model has been intensively studied as its ground state is exactly shown to be a QSL with Majorana quasiparticles fractionalized from quantum spins [1]. Although a lot of attempts have been devoted to the observations of the fractional quasiparticles, the experimental identification remains elusive. This is due to the difficulty on observing each quasiparticle separately using experimental probes.

In this study, to observe the fractional excitations, we focus on the time evolution of their non-equilibrium dynamics. In our previous work, we examined the magnetic-field effect on the ferromagnetic and antiferromagnetic Kitaev models using the Hartree-Fock approximation in the Majorana fermion representation [2]. Here, we examine the transient magnetic dynamics yielded by the magnetic-field quench by extending the previous work. In the Kitaev model, a quantum spin is fractionalized into low-energy localized Majorana fermions and high-energy itinerant ones. We find that two kinds of Majorana fermions are observed separately in distinct time-scales in the time evolution of the magnetization; the low-energy localized Majorana fermions survive as long-lived excitations whereas the high-energy itinerant ones are damped in the early stage.

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Ab initio studies on superconductivity and inhomogeneity in Hg-based cuprate superconductor

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Despite many experimental and theoretical studies on high-T_c cuprates, understanding its rich physics remains one of the most important outstanding problems in materials science. In particular, charge order found in underdoped regions has been recently established as a ubiquitous feature and their competitions with superconductivity are attracting great attentions, where the simple Hubbard model on a square lattice has often been studied and recent progress on the numerical accuracy has allowed to reach an overall consensus. However, neither the period of the spin/charge order nor its dominance over homogeneous superconductivity is consistent with experimental observations [1-3]. Therefore, realistic first-principles studies are highly desirable.

In this study [4], we solved an *ab initio* low-energy effective Hamiltonian of $HgBa_2CuO_{4+\delta}$ which has been recently derived without any adjustable parameters[5]. To solve the Hamiltonian accurately, we employed a many-variable variational Monte Carlo method [6] combined with a tensor-network and/or the power Lanczos method together with the energy-variance extrapolation for a controlled calculation. Our results quantitatively reproduce experiments including a wide hole-density region of superconducting phase while competing with a period-4 charge order near the hole density $\delta \sim 0.1$ consistently with recent X-ray scattering measurements. To understand the superconducting amplitude and stability, crucial role of realistic off-site interactions is revealed. Furthermore, we find that the enhancement of superconductivity is well correlated with charge fluctuations rather than spin fluctuations.

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Resummation of diagrammatic series with zero convergence radius for the unitary Fermi gas

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Feynman diagrams are powerful tools for studying various fields of physics. Still, the analysis usually involves approximations, because only some types of diagrams or low-order diagrams are considered there. However, the Monte Carlo method for unbiased sampling of Feynman diagrams has been recently developed[1-3]. On the other hand, the diagrammatic series sometimes have zero radius of convergence. The question is whether it is still possible to make accurate predictions by summing up Feynman diagrams.

Here we report high-precision results obtained by the bold-line diagrammatic Monte Carlo method for the unitary Fermi gas with zero convergence radius[4]. We derive the large-order asymptotic behavior of the diagrammatic series, and we give mathematical arguments and numerical evidence for the resummability of the series by a specifically designed conformal-Borel method that incorporates the large-order behavior. Combining this new resummation method with diagrammatic Monte Carlo evaluation up to order 9, we obtain new results for the equation of state, which agree with the ultracold-atom experimental data, except for the 4-th virial coefficient for which our data point to the theoretically conjectured value. I will also report our accurate results of Tan's contact[5].

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Effect of Coulomb Interaction in Seebeck Coefficient of Organic Dirac Electron System α-(BEDT-TTF)$_2$I$_3$

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The organic conductor -(BEDT-TTF)$_2$I$_3$ (α–ET) has a massless Dirac electron (massless DE) phase in its pressure-temperature phase diagram at high temperature and high pressure. In massless DE phase, α–ET shows unique physical properties particular to Dirac electron (e.g. quantum conduction) [1]. When the inversion symmetry is broken below critical temperature T_{CO} and pressure P_C, α–ET becomes a charge ordered (CO) phase due to the nearest neighbor coulomb interaction [2]. In massless DE phase, a velocity renormalization and excitonic fluctuation due to the long range coulomb interaction have been observed by NMR measurement [3]. Thus, electronic correlation effect plays significant roles in each phase in α–ET.

In this study, we focus on an anomalous pressure-temperature dependence of a Seebeck coefficient S(T) in α-ET [4, 5]. S(T) in $P > P_C$ has a positive value, and shows peak structure at T = 50K, and linearly decreases toward T = 0K as temperature decreases. On the other hand, in $P < P_C$, S(T) being positive in massless DE phase shows a peak at $T \sim T_{CO}$, and sharp drop of the value with sign inversion. The mechanism of these unique temperature dependences in S(T) have not been elucidated.

In the present study, we will calculate the Seebeck coefficient S(T) using Nakano-Kubo formula and semi classical formula, and aim to elucidate the mechanisms of these unique behaviors. The electronic correlation in S(T) is investigated using extended Hubbard model which describes the electronic structure of α-ET. We treat the chemical potential carefully, since the chemical potential in Dirac electron system is sensitive to the carrier doping and electron-hole asymmetry [6], and S(T) is sensitive to the chemical potential [7].

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Time-reversal symmetry breaking superconductivity in hole-doped monolayer MoS_2

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Time-reversal symmetry (TRS) breaking superconductors have attracted much attention in their intriguing features. Although no TRS breaking spin-singlet states have been observed so far, possible TRS breaking spin-singlet state has been proposed in several candidate materials, such as Fe-based superconductors [1]. These TRS breaking states are commonly characterized by their multi-band features with potential frustration in the relative phase among their Cooper pairing components, leading to an intermediate phase in between the range, $[0, \pi]$. Consequently, spontaneous TRS breaking superconductivity emerges [2].

In recent years, the layered transition-metal dichalcogenides (TMDCs) have extensively been investigated both experimentally and theoretically as a new platform for exotic superconductivity in context of spin-orbit physics. In particular, it has been suggested that the hole-doped TMDCs have a richer variety of pairing states than the electron-doped one, because the valence bands have much characteristics originating from Mo d orbitals with relatively strong spin-orbit coupling (SOC) [3,4]. We examined theoretically the Cooper-pair symmetries within s waves that can be realized in hole-doped monolayer MoS_2 [4], in which we introduced the multi-orbital gap functions; the conventional spin-singlet ψ in the Γ pocket, spin-triplet orbital-singlet d_z, and spin-singlet orbital-triplet D_z in the K and K′ pockets.

In the present study, we have further investigated the nature of the pairing states in the superconducting phase. Figure 1(a) shows the doping ($x = 2 - n$, n being the electron density per unit cell) dependence of T_c and the Cooper-pair components for $U = 0.5, J = -U/1.7$, and $\lambda = 0.073$ eV. The red, green and blue arrows represent ψ, D_z and d_z in the complex plane, respectively, and ϕ_1 is the relative phase between ψ and d_z. The change of the Fermi-surface topology and the relative phase of the parings near $x \sim 0.1$ is shown in Fig. 1(b). The TRS breaking phase appears inside the TRS preserving phase, in which $\phi_1 \neq 0, \pi$. This pairing is triggered by the Lifshitz-transition realized at $x \sim 0.1$ (Fig. 1(b)). Note that this intriguing pairing can emerge only in the presence of SOC, because without SOC, ψ, D_z, and d_z cannot hybridize with each other by symmetry. We will also discuss the densities of the finite spin and orbital angular momentum in the TRS breaking phase in the momentum space.

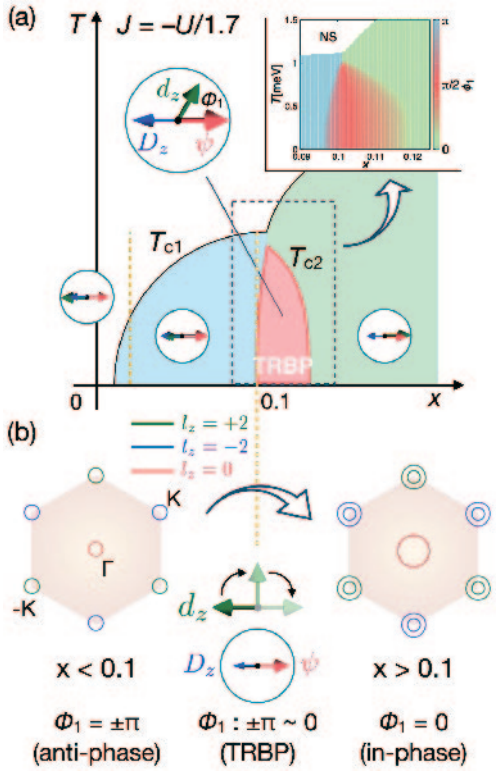

Figure 1: (a) Phase diagram of the doping x vs. temperature T for $U = 0.5$, $J = -U/1.7$, and $\lambda = 0.073$ eV. ϕ_1 is the relative phase between ψ and d_z. (b) Change of the Fermi-surface topology and the relative phase of the pairings near $x \sim 0.1$.

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Spin-charge coupled phenomena in a chiral soliton lattice

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Chiral magnets often show interesting properties associated with their peculiar spin structures. A typical example is a chiral soliton lattice (CSL), which was found in monoaxial chiral magnetic conductors $CrNb_3S_6$ [1] and $Yb(Ni_{1-x}Cu_x)_3Al_9$ [2]. These compounds show a helimagnetic state at zero field and turn into the CSL in a magnetic field perpendicular to the helical axis (Fig. 1). As the magnetic field increases, the spatial period of the CSL increases and finally the system relaxes into a forced ferromagnetic state (FFM). While itinerant electrons might play an important role in the electronic and magnetic properties in these chiral states, most of the previous theoretical studies were focused on effective localized spin models.

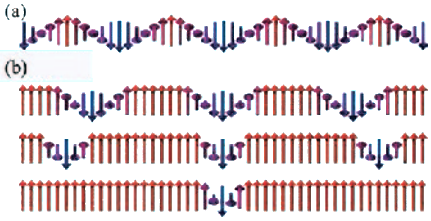

Fig. 1: Schematic pictures of (a) a chiral helimagnetic state, (b) chiral soliton lattices (CSLs).

In this study, we investigate a minimal itinerant electron model, a one-dimensional Kondo lattice model with the Dzyaloshinskii-Moriya interaction, by variational calculations for the ground state and by Monte Carlo simulations at finite temperatures. We show that the model exhibits peculiar behavior in an applied field, which was not found in the localized spin models. In particular, we find that the spatial period of CSL can be locked at particular values dictated by the Fermi wave number (Fig. 2) [3]. The result suggests the possibility of spontaneous formation of the CSL even at zero field. We also show that the CSL exhibits nonlinear negative magnetoresistance, which is closely related to the soliton density (Fig. 3) [4].

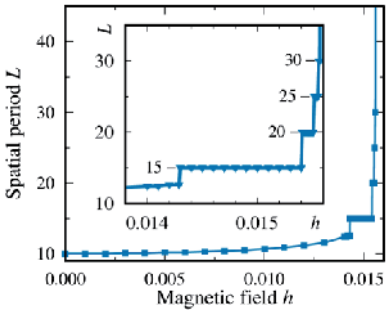

Fig. 2: Lock-in of the spatial period of CSL in a magnetic field.

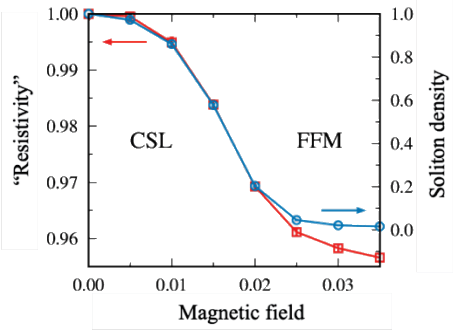

Fig. 3: Nonlinear negative magnetoresistance which is proportional to the soliton density.

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Numerical study of magnetic hedgehog crystals in itinerant chiral magnets

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Chiral magnets have attracted much attention due to the interesting properties associated with their peculiar spin structures originating from the antisymmetric exchange interaction called the Dzyaloshinkii-Moriya interaction. For example, among the *B*20-type compounds, MnSi and MnGe show 2D skyrmion and 3D hedgehog crystals, respectively, both of which are characterized by three wave numbers (3Q). These peculiar spin structures induce an interesting quantum transport called a topological Hall effect [1]. In addition, a new chiral spin texture characterized by four wave numbers, the 4Q hedgehog crystal, has been reported in $MnSi_{1-x}Ge_x$ [2]. Although such systems are metallic and the coupling between spin and charge should be important, there is no theoretical study including the effect of itinerant electrons for the chiral multiple-Q states.

In the present study, in order to clarify the stability of the chiral multiple-Q states in the 3D systems, we study an effective spin model including the effect of itinerant electrons and spin-orbit interaction by variational calculations and Monte Carlo simulations. We find several 3D chiral spin textures, including the skyrmion and hedgehog crystals with the 3Q and 4Q vectors shown in Fig. 1. We also discuss the behaviors of such multiple-Q spin textures in a magnetic field.

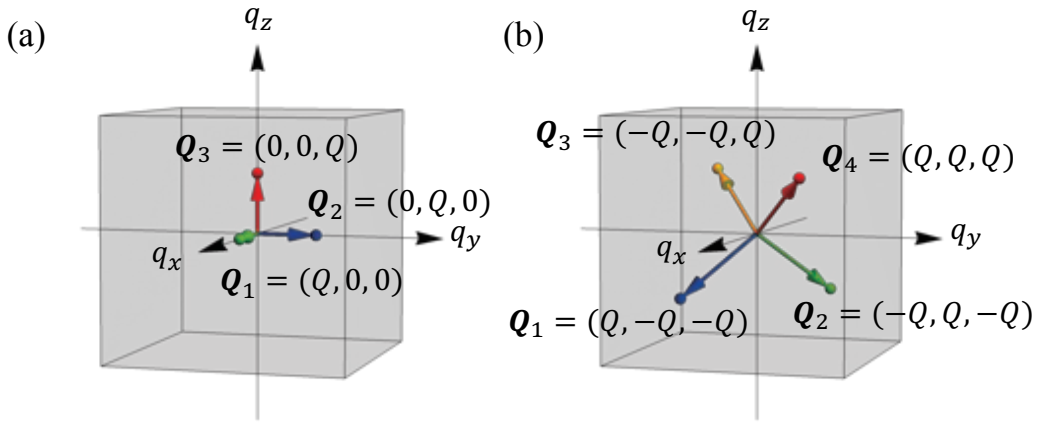

Fig. 1: Examples of the ordering vectors for (a) 3Q and (b) 4Q states.

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Symmetry Indicators for Topological Superconductors

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Many people are making efforts to investigate the relationships between topology and symmetry, especially searching for topological crystalline insulators (TCI) and topological superconductors (TSC). L. Fu and C. L. Kane proposed the first efficient way to discover TI, called Fu-Kane formula [1], which is applicable to inversion symmetric systems. Recently, there have been fundamental advances in the method of symmetry indicators [2] and in a similar formalism, which provide an efficient way to diagnose the topology of band insulators and semimetals based on the representations of valence bands at high-symmetry momenta. This scheme can be understood as a generalization of the Fu-Kane formula that computes the topological index in terms of inversion parities to arbitrary space groups and a wider class of topologies including higher-order ones. It formed the basis of recent extensive material searches based on the density functional theory (DFT) calculation by several groups that resulted in the discovery of an enormous number of new topological materials [3-5]. Up to this moment, however, symmetry indicators are applicable only to insulators and semimetals. If one wants to apply this method to SCs, one must examine the representations in the band structure of the Bogoliubov-de Gennes (BdG) Hamiltonian including a gap function. In fact, this is the approach taken in Ref. [6] that recently extended the symmetry indicators to the 10 Altland-Zirnbauer symmetry classes. However, this is not ideal because such a band structure is not available in the standard DFT calculation. Furthermore, in this way, the total number of bands that have to be taken into account can be huge unless one uses an effective tight-binding model.

In this work, we further develop the theory of symmetry indicators exclusively designed for SCs. It enables us to determine the topology of SCs based on the representations of a finite number of bands below the Fermi surface in the normal phase, although one still has to assume a symmetry transformation property of the gap function [7].

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Anomalous energy transfer between electrons and phonons in photoexcited metals

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The energy relaxation dynamics of photoexcited metals has been usually interpreted based on the two-temperature model (2TM), where the electron and phonon temperatures are assumed to be defined at any time. However, the assumption behind the 2TM is questionable because the effects of electron-electron (e-e) and phonon-phonon (ph-ph) collisions would not be strong enough to keep the quasiequilibrium distribution and that of electron-phonon (e-ph) collisions would be strong enough to disturb the quasiequilibrium.

We thus study the relaxation dynamics in electron-excited metals by using the Boltzmann equation with e-e, e-ph, and ph-ph collisions [1]. Figure 1(a) shows the time-evolution of the excess energies of electron, LA phonon, and TA phonon. Most of the electron energy is transferred to the LA phonon system through e-ph collisions in the initial relaxation. In a meanwhile, the energy transferred is redistributed through ph-ph collisions to reach thermal equilibrium, yielding an overshoot of the LA phonon energy at 0.2 ps. Interestingly, the electron energy decays quite slowly before reaching thermal equilibrium (Fig. 1(b)). This anomaly can occur as a result of the *backward energy flow* from LA phonons to electrons (Fig. 1(c)). Similar slow dynamics has been observed in the final stage of relaxation for other systems [2,3]. The present study suggests that the appearance of backward energy flow would be an indicator for thermalization [4].

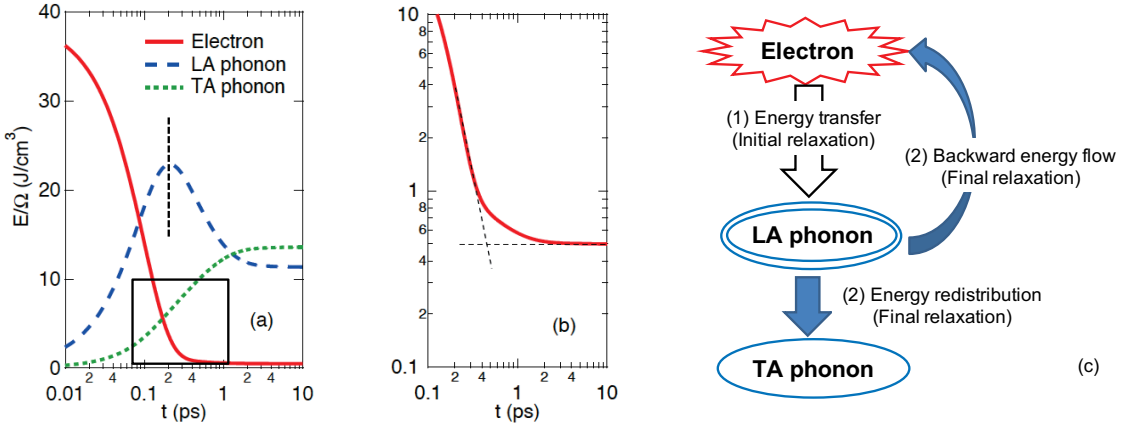

Fig. 1: (a) The time-evolution of the excess energies in an electron excited metal. (b) The magnified view of the electron energy. (c) Schematic illustration of the relaxation processes.

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Strong-coupling formula of momentum-dependent susceptibilities in dynamical mean-field theory

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The dynamical mean-field theory (DMFT) and its combination to the density functional theory (DFT+DMFT) have been extensively applied to strongly correlated models and materials. For computing two-particle responses $\chi(\boldsymbol{q})$, one needs to solve the Bethe-Salpeter equation, which demands large computational cost compared to the single-particle excitations. For this reason, it is difficult to perform susceptibility calculations for realistic materials with *d* and/or *f* electrons.

Recently, we derived a simplified formula for $\chi(\boldsymbol{q})$ that can be solved at a considerably lower cost [1]. The formula presents the features listed below:

- The formula has an RPA-like form, and calculations are quite easy.
- The derivation of the formula exploits a strong-coupling feature of the vertex function, but numerical calculations demonstrate surprisingly wider applicability including weak-coupling region.
- Momentum dependence is characterized by an effective intersite interactions $I(\boldsymbol{q})$. In the strong-coupling limit, $I(\boldsymbol{q})$ is reduced to the well-known formulas such as the kinetic exchange interaction and the RKKY interaction. Hence, our formula also offers a way to estimate $I(\boldsymbol{q})$ in first-principles calculations.

In the presentation, we present the details of the formula and its application to multiorbital models.

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Quantum oscillations in topological Kondo insulator

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One of the most puzzling recent experimental discoveries in condensed matter physics has been the observation of quantum oscillations in insulating materials SmB_6 and YbB_{12} [1,2]. Our understanding of quantum oscillations is rooted in the existence of a Fermi surface; electron bands, which form the Fermi surface, form Landau levels in a magnetic field. When the magnetic field strength is changed, the energy of these Landau levels changes which lead to an oscillatory behavior in almost all of the observable properties. However, SmB_6 and YbB_{12} are strongly correlated *f* electron systems for which a gap develops due to a hybridization between conduction electrons and strongly correlated *f* electrons, and thus a large resistivity at low temperatures can be measured. Thus, we can expect that SmB_6 and YbB_{12} do not possess a Fermi surface, thus there are no electrons, which can form Landau levels close to the Fermi energy. On the other hand, SmB_6 and YbB_{12} are both good candidates for topological Kondo insulator. Naturally, the question arises, if these quantum oscillations can be due to the interplay between non-trivial topology and strong correlations.

We here answer this question by showing results of dynamical mean field theory in a magnetic field for a two dimensional topological Kondo insulator. We demonstrate that the gap closing, described for a noninteracting continuum model with momentum dependent hybridization [3], persists for a topological Kondo insulator on a two dimensional (2D) lattice, see Fig. 1. Furthermore, we demonstrate that the amplitude of quantum oscillations is strongly enhanced due to correlations, which makes them easily observable in quantities like magnetization and resistivity over a wide range of magnetic fields before the magnetic breakdown occurs.

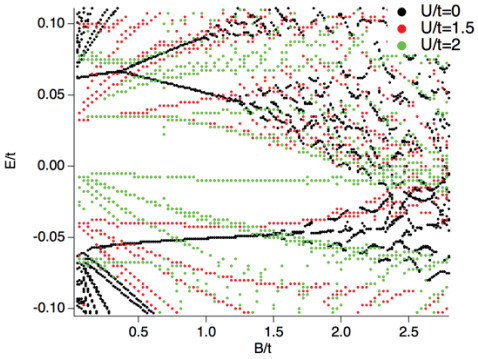

Figure 1: Comparison of energy levels in noninteracting and interacting model for different magnetic fields.

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For more information see: arXiv:1901.05099

Quantum spin liquids in the pyrochlore S=1/2 Heisenberg model with Dzyaloshinskii-Moriya interactions

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The discovery of novel quantum states of matter such as spin liquids stimulates the investigation of new materials and model systems. Recently it has been suggested that a new quantum spin liquid phase might occur in pyrochlore iridates [1], materials with notably strong spin-orbit coupling. In order to quantify this statement, we numerically investigate the quantum S=1/2 Heisenberg model with Dzyaloshinskii-Moriya interactions on the pyrochlore lattice. By starting from a projection of the pyrochlore lattice along the (001) direction (the 2 dimensional checkerboard lattice), we benchmark our many-variable variational Monte Carlo (mVMC) [2, 3] results to exact diagonalization (ED) [4] and iPEPS [5] data. By extending the lattice into the third dimension we allow for a transition between the 2 dimensional checkerboard and the 3 dimensional pyrochlore physics, and open the door for detailed investigations of their ground state properties.

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P56

The role of exchange interactions on spin reorientation transition of $Nd_{0.5}Dy_{0.5}FeO_3$: A first principle study

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The rare-earth orthoferrites ($RFeO_3$) which are known for their spin-reorientation and other interesting properties like magneto-dielectric effect show a large Neel temperature of 700 K, below which the Fe^{3+} spins order as G-type antiferromagnet in the configuration Γ_4 (Gx,Ay,Fz). Magnetic properties and electronic structures of rare-earth orthoferrite $Nd_{0.5}Dy_{0.5}FeO_3$ have been studied by performing accurate first principle calculation based on density functional theory. Among the various possible magnetic configurations of Fe^{3+} spins with the frozen Nd/Dy 4f states, the G-type ordering emerges as the ground state. Both, $NdFeO_3$ and $DyFeO_3$, order in entirely different magnetic configurations. From our calculations it is found that C-type magnetic structure emerges as the lowest energy state of Nd^{3+}/Dy^{3+}, which is well in agreement with experiments. The spin-reorientation and the ground state of Fe^{3+} moments are evaluated using non-collinear calculations with spin-orbit coupling. With inclusion of 4f states of Nd/Dy, the Γ_2 structure emerges as lowest energy in the Fe^{3+} spins which is thereby consistent with experiment and symmetry analysis. Estimation of exchange interactions by mapping the system to Heisenberg model yields a competing Nd-Fe and Nd-Dy and Dy-Dy exchange interactions in comparison to much smaller Dy-Fe and Nd-Nd interactions. Hence, it is clear that the Nd^{3+} -Fe^{3+} and Nd^{3+} -Dy^{3+} exchange interactions play a dominant role in large polarization of the rare earth ions which prevent independent ordering of the Nd^{3+} - Dy^{3+} moments.

Poster Presentations – Section C

P57

Inversion and Magnetic Quantum Oscillations in Kondo Insulators

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Jawaharlal Nehru University, New Delhi

The occurrence of magnetic quantum oscillations in Samarium hexaboride (SmB6), a Kondo insulator, caused a stir in condensed matter community because it is not expected to occur in insulators [1, 2]. The periodic oscillations in magnetization with respect to the (inverse) magnetic field is known as de Haas-van Alphen (dHvA) effect, which is considered as a hallmark of the metallic systems and a direct probe to the Fermi surface [3, 4]. The dHvA oscillations in SmB6 forced us to reexamine and reconsider the underline working principle. In this regard, some interesting theoretical studies are proposed but still, this recalls for clear understanding.

In this poster, I would present our theoretical study of quantum oscillations in Kondo insulators by considering basic models, Kondo lattice model and symmetric periodic Anderson model, all at half-filling on bipartite lattices. Using a canonical representation of electrons invented by Kumar [5], we construct a self-consistent theory of spin and charge dynamics that appropriately describes the Kondo insulating state and gives the quantum oscillations of magnetization as a general bulk property. We get these oscillations due to inversion of charge quasiparticles dispersion whose effective chemical-potential surface they measure. These quasiparticles are gapped and occupy half of the bulk BZ [6, 7].

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Dynamics of the magnetic polaron

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The magnetic polaron is a quasiparticle that appears in the low-density limit of the Kondo Lattice Model. It is an electron dressed by a cloud of magnons and can be thought of as an opposite limit to the Kondo problem (where a single localized spin is screened by electrons). We discuss the eigenstates of the Correlated Kondo Lattice Model in the low-density limit and show that additional states appear: a flat doublon band without any dispersion; and a triplet-coupled polaron band. The doublon is a bound state of two electrons otherwise known from the Hubbard model, but appears here even for $U = 0$, acquiring a dispersion for $U > 0$. We discuss the consequences of these states for real-time dynamics and spectroscopies using the time-dependent density matrix renormalization group (t-DMRG) in one dimension.

Superconductivity in quasiperiodic systems

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Quasicrystal can be a platform of novel electronic properties because of its self-similar but aperiodic crystal structure. Early studies on quasiperiodic systems focused on noninteracting electrons, which indeed show various anomalous properties distinct from those in periodic systems, while recent experiments [1,2] have advanced our interests to interacting electrons in quasiperiodic systems.

In this work, we theoretically study quasiperiodic superconductors, which were indeed discovered in recent experiment [2]. Because of the lack of the Fermi surface, fundamental questions are how Cooper pairs are formed and what property differs from that of periodic superconductors. We studied these issues by introducing a simple theoretical model, the attractive Hubbard model on a two-dimensional Penrose structure.

Through numerical simulations on this model, we find a superconductivity at low temperatures. Reflecting the aperiodicity of the Penrose structure, the superconducting state exhibits a spatial inhomogeneity, which however conforms with the five-fold rotational symmetry and self-similarity. [3] We further study the effect of magnetic field on the quasiperiodic superconductors, where we find a novel superconducting state with a spatially alternating sign of the superconducting order parameter. [4]

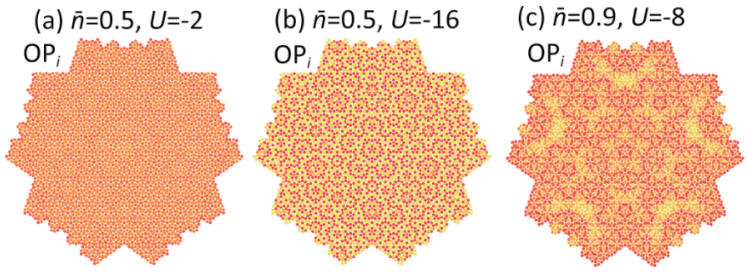

Fig.: Spatial pattern of onsite superconducting order parameter for various choices of the average electron density n and attraction U, calculated on a 4181-site Penrose cluster. Large (small) amplitude is colored by red (yellow).

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Magneto-optic study of thermally driven ferrimagnet-helimagnet transition in a chiral-polar magnet

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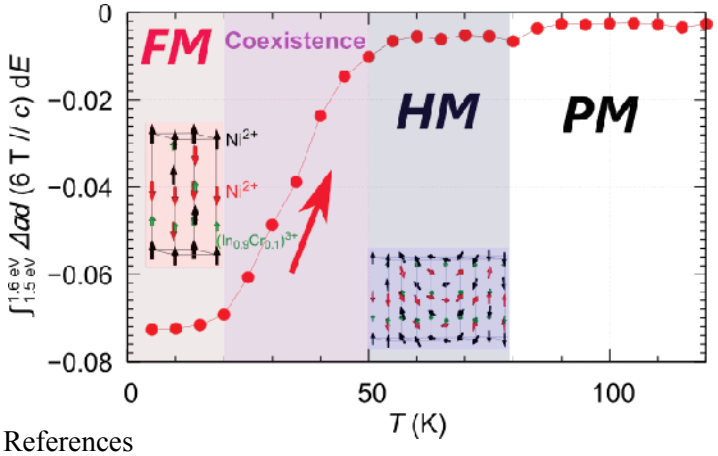
A chiral polar magnet Ni_2InSbO_6 (NISO), which belongs to space group *R*3, was first synthesized in 2013 [1,2]. It has a long-periodic helimagnetic (HM) ground state with a modulation vector perpendicular to crystallographic axis [1]. Recently, we have synthesized $Ni_2In_{0.9}Cr_{0.1}SbO_6$ (NICSO), where magnetic Cr^{3+} ions are partially substituted for nonmagnetic In^{3+} ions. HM ground state in NICSO becomes commensurate ferrimagnetic structure in a magnetic field of a few tesla, while HM state is stable up to around 20 T in NISO [3, 4].

Here we present a magneto-optic study of the magnetic phase transition in NICSO. We have observed that a magnetic field suppresses the absorption intensity around 1.55 eV at 4.2 K. This negative magnetochromism arises from the spin-dependent oscillator strength of intra-atomic *d-d* excitation from $^3A_2$ ground state to ^1E excited state of Ni^{2+} ion with d^8 electronic configuration. The magnetochromism is found to diminish around 50 K (see Figure), below the Neel temperature 84 K. It indicates that the FM state at low temperatures is thermally destabilized and turns to HM state, similar to the case of skyrmion crystal phase in some chiral or polar noncentrosymmetric helimagnets.



Temperature dependence of magnetochromism around 1.55 eV in NICSO. Vertical axis corresponds to the change in the absorption intensity around 1.55 eV. PM denotes paramagnet. Insets show schematically illustrated magnetic structure.

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Quantum Criticality in the Two-Dimensional Periodic Anderson Model

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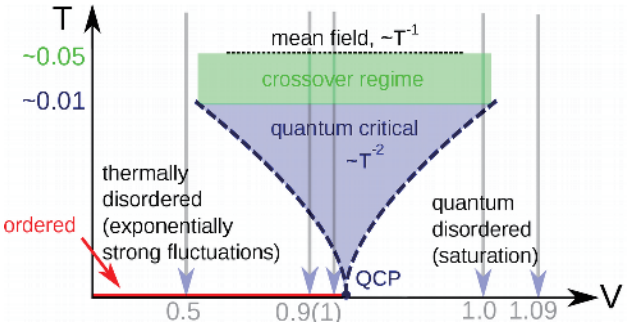
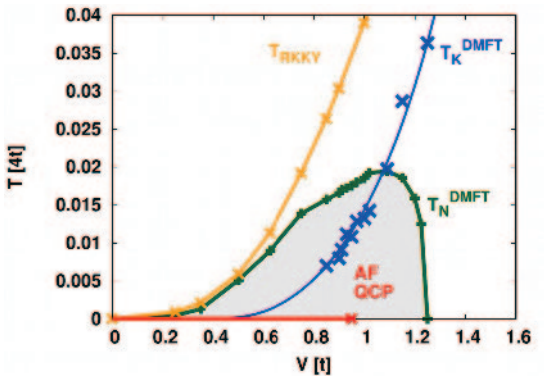
Despite the fascinating physical phenomena accompanying a quantum critical point, e.g. the exhibition of non-Fermi liquid behavior, a general theory for quantum phase transitions is still lacking.

In my poster presentation, I will show a step forward by analyzing results from the dynamical vertex approximation (DΓA), a cutting-edge quantum field theoretical method including temporal as well as spatial correlations. Within this framework, I will analyze the fundamental model of strongly correlated heavy fermion compounds, the perdiodic Anderson model, in two dimensions. By varying the hybridization strength of localized f-electrons and itinerant d-electrons, and a careful analysis of response functions, one can trace the change in the ground state from an antiferromagnet at low hybridizations to a paramagnetic Kondo insulating phase, resembling the famous Doniach phase diagram. Eventually, I will show the evolution of the (classical and quantum) critical exponents of the magnetic susceptibility, which are changing from the one of free spins $\gamma = 1$ to $\gamma = 2$ in the quantum critical regime.





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Two-dome superconductivity in FeS induced by a Lifshitz transition

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Recently, two superconducting domes in the temperature-pressure phase diagram for FeS have been observed [1]. FeS has a tetragonal structure and superconducts with the critical temperature T_c = 4.7K at ambient pressure. The superconductivity is suppressed at approximately 4 GPa, and the second dome appears from 5 GPa to 22 GPa. Since it has been reported that a structural phase transition from tetragonal into hexagonal occurs around 7 GPa, it has been unclear what causes the reentrant superconductivity.

In this study, we calculate the superconducting order parameter with density functional theory and spin fluctuation theory calculations using the structure obtained from experiment [2]. We find that the pairing strength decreases up to 4.6 GPa and increases again from 4.7 GPa to 5.5 GPa, in agreement with experiment. The superconducting gap symmetry changes at 4.7 GPa from d wave to nodeless sign changing s wave. Detailed analysis of the spin susceptibility allows us to link the change of order parameter to the additional Fermi surface presents after the Lifshitz transition.

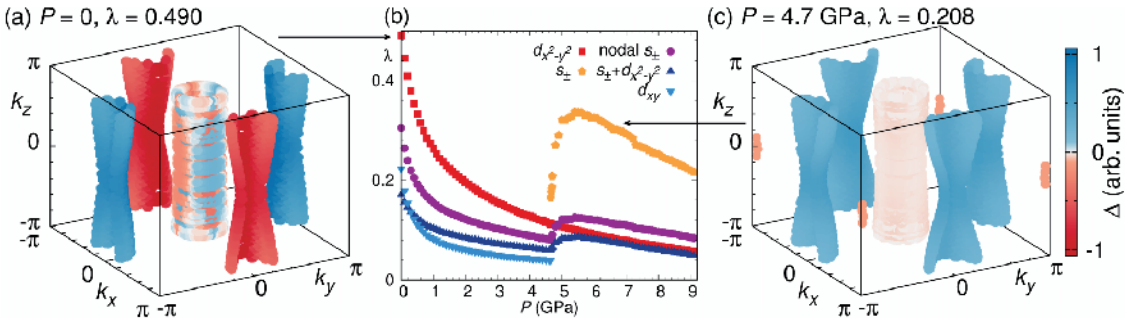

Fig. 1: Leading gap functions for FeS at (a) ambient pressure and (c) P = 4.7 GPa. (b) Leading eigenvalues λ of the linearized gap equation as function of pressure.

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Dynamical susceptibility in DMFT: a sparse QMC sampling approach

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Computing dynamical susceptibility in dynamical mean-field theory (DMFT) is challenging due to large computation time and massive memory consumption in dealing with two-particle Green's function. Recently, some of us and co-workers have proposed a compact representation of two-particle Green's functions [1] based on the "intermediate representation" (IR) basis [2]. In this compact representation, the data size of two-particle Green's functions grows only logarithmically with inverse temperature.

In this talk, we discuss a new technique for the efficient quantum Monte Carlo (QMC) sampling of two-particle Green's functions in the framework of DMFT. The sampling is performed only at a sparse set of Matsubara frequencies, dramatically reducing the computational costs and memory footprint. We demonstrate that the correct low-/high-frequency structures can be recovered from the sampling data.

The sparse sampling can be used for the calculation of dynamic susceptibilities, after inversion of the Bethe-Salpeter equation. We present results in the context of the BEC to BCS crossover [3, 4] in the vicinity of the excitonic condensation in the two-band Hubbard model [5]. We also discuss future applications of this technique to *ab-initio* calculations of dynamical susceptibility and diagrammatic extensions of DMFT.

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Machine learning study of photoexcited states in the half-filled one-dimensional extended Hubbard model

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Photoinduced nonequilibrium states can provide new insights into the dynamical properties in strongly correlated electron systems. One of the typical and extensively studied systems is the half-filled one-dimensional extended Hubbard model (1DEHM). Here, we propose that the supervised machine learning (ML) can give useful information for characterizing the photoexcited state in 1DEHM [1]. Using entanglement spectra as a training dataset, we construct the neural network. Judging from the trained network, we find that the quantum state driven by driving pulse has bond-spin-density wave (BSDW) order for $U \lesssim 2V$, where U (V) is the on-site (nearest-neighbor) Coulomb interaction. We separately calculate the time evolution of order parameters and find that the order parameters of BSDW are actually enhanced by photoexcitation as predicted by ML. Interestingly, the enhancement of the BSDW order in the photoexcited states for the 1DEHM has never been reported previously, despite the extensive studies so far, thus demonstrating the advantage of ML to assist characterizing photoexcited quantum states.

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Possible Enhancement of Coercivity in Rare-Earth Permanent Magnets on the Verge of a Valence Transition

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$CeCo_5$ and $CeCu_5$ crystalize $CaCu_5$-type hexagonal structure, which is the same structure as a prototypical commercial rare-earth permanent magnet $SmCo_5$. $CeCo_5$ orders ferromagnetically below the Curie temperature T_C = 649 K, and Ce is tetravalent [1]. $CeCu_5$ becomes antiferromagnet below the Néel temperature T_N = 3.9 K, and is a heavy fermion compound [2]. Thus, Ce is trivalent. Therefore, one can expect that a valence transition in Ce would emerge induced by Cu substitution for Co in $CeCo_5$. To investigate the influence of valence fluctuations to the ferromagnetic property, we grew poly-crystalline samples of $Ce(Co_{1-x}Cu_x)_5$. We measured magnetization by SQUID magnetometer (MPMS3, Quantum Design) in the temperature range 2 -300 K. Reflecting a ferromagnetic ordering, magnetization curves for $x \leq 0.6$ exhibit clear hysteresis loops. Ferromagnetic phase as a function of x is consistent with the previous report [3]. No extrinsic pinning centers are observed in our samples. Intrinsic coercivity H_c is strongly enhanced by Cu substitution and has a maximum at x = 0.3. More interestingly, H_c for $x \sim 0.5$ exhibits steep increase at low temperatures, whereas that for $x \sim 0.3$ is monotonically enhanced with decreasing temperature. These results imply the enhancement of H_c on the verge of valence transition induced by Cu substitution or temperature in $Ce(Co,Cu)_5$. Implications on variants of crystal lattices are discussed.

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Quantized Excitation Spectra by Confinement in (Quasi-)One-Dimensional S=1 Quantum Spin Systems

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The infinite time-evolving block decimation algorithm is applied to calculate the dynamical spin structure factor (DSF) of (quasi-)one-dimensional (q1D) S=1 quantum spin systems. We first consider the q1D S=1 antiferromagnetic Heisenberg spin system with single-ion anisotropy and bond alternation [1]. We find that the staggered field arising from the weak interchain interaction changes the excitation continuum originating from magnons into the quantized spectra. When the single-ion anisotropy is negatively strong, the energies of the quantized spectra agree well with the negative zeros in the Airy function (NZAF). This quantized magnon spectra is a counterpart of the quantized excitation spectra caused by the spinon confinement in the q1D S=1/2 antiferromagnets, which has been recently observed in the inelastic neutron scattering (INS) experiments [2,3]. We further show that the quantized excitation spectra appear near the phase boundary between the Haldane and Neel phases in the phase diagram. We next consider the S=1 ferromagnetic (FM) Ising spin chain with negative single-ion anisotropy in magnetic fields [4]. When the transverse magnetic field is applied, both the ΔS=2 excitation continuum and the one-magnon mode appear in the low-lying excitation. When the longitudinal magnetic field is further applied, the ΔS=2 excitation continuum changes into the quantized excitation spectra as shown in Fig. 1. The quantized ΔS=2 excitation spectra originate from confinement of two domain walls, each of which carries ΔS=1. The quantized excitation energies agree with the NZAF. We expect the obtained quantized excitation spectra to be detected by the INS experiments.

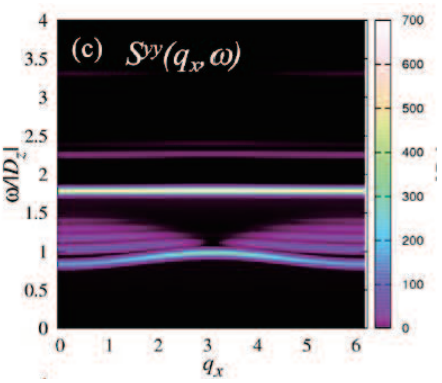

Fig. 1: DSF of the S=1 FM Ising spin chain in magnetic fields. Quantized excitation spectra below one-magnon mode.

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Topological Transition in Hard-Core Bosonic Haldane Model

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The topological Haldane model on two-dimensional honeycomb lattice is well known as the first example where it can exhibit quantum Hall effect without magnetic fields [1]. This model breaks the time-reversal and sublattice symmetries due to the second-neighbor hopping with a phase and the alternating chemical potential, leading to the non-trivial Chern number. This non-zero Chern number indicates the presence of the chiral edge state and the non-zero Hall conductance. Inspired by this study, recent theoretical studies on topological states have been extended to no-fermion systems, e.g., bosonic systems [2]. Interestingly, the recent study has shown that even the bosonic systems exhibit non-trivial topological number.

Here, we consider a hard-core boson instead of fermion and boson as a quantum object on the Haldane model. The hard-core boson has the same commutation relation as one-half spin, i.e., on-site anti-commutation and inter-site commutation. The Jordan-Wigner transform of one-half spin to fermion causes the many-body interaction in two-dimensional systems. Therefore, we can clarify not only the quantum statistical effects but also the effects of interaction on the topological state in this model. To break the time-reversal symmetry, we introduce a second-neighbor hopping term with a phase depending on number operator at the neighboring sites, which corresponds to the scalar chirality of three spins. Additionally, we also introduce an anisotropy in the lattice to break the sublattice symmetry. As the result, we have found the signature of topological transition in this model. Our study also indicates a possibility of new topological states in quantum spin systems.

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Large-scale dynamical simulation of Hubbard model

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[3]*Department of Physics, University of Virginia, Charlottesville, VA*
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[5]*Quantum Condensed Matter Division and Shull-Wollan Center, Oak Ridge National Laboratory, Oak Ridge, TN*

Weak Mott insulators emerge from 5d electron systems with strong spin-orbit couplings. Coulomb repulsion (U) between electrons in 5d orbitals is not strong enough to suppress charge degrees of freedom completely. For example, the charge gap is comparable to the magnon-band width for strontium iridates. Such electron systems can be described by the Hubbard model with an intermediate U, which would be in the crossover regime between Slater and Mott insulators. Reliable calculation for the intermediate-U region is theoretically challenging because of the lack of a small parameter in the model. We have developed a new numerical approach that enables large-scale calculation (with more than 10^4 sites) of dynamical quantities at finite temperatures in the broad-U region (Fig. 1). In our approach, the sampling of auxiliary vector fields from the Boltzmann distribution and the real-time dynamics of the density matrix are successfully combined. As an application of the newly developed method, we calculated the dynamical spin structure factor, targeting 5d electron systems. Our calculation accounts for experimental results of relevant materials such as iridates. Importantly, our approach is applicable to various systems without any restrictions on the type of hopping, the type of lattice, and electron filling. The broad U region is accessible up to the temperature comparable to the charge gap.

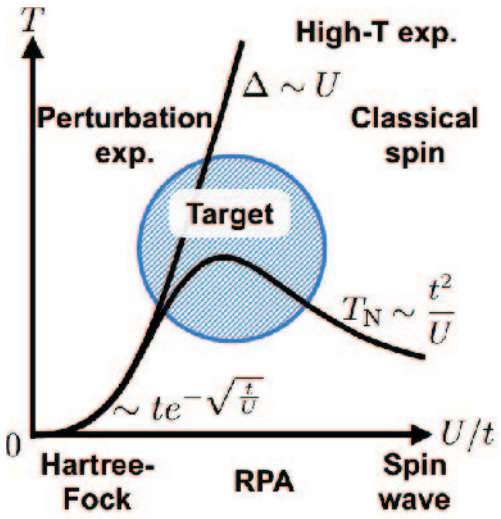

Fig. 1: Target region and valid approaches in the parameter space of interaction strength (U/t) and temperature (T).

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Ground-state phase diagram of the extended Kitaev-Γ model on a honeycomb lattice

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Since the features of the Kitaev spin liquid (KSL) have been reported in the inelastic neutron scattering experiments on a honeycomb-lattice magnet, α-$RuCl_3$[1,2], this compound has been the focus of intensive research. The proper model for α-$RuCl_3$ have been much discussed so far. It has been pointed out that not only the Kitaev interaction (K) but also the symmetric off-diagonal interaction (Γ) acting on the nearest-neighbor effective spins is important to explain the characteristic features of α-$RuCl_3$[3,4]. The recent numerical calculations for the K-Γ model on a honeycomb lattice have pointed out that a quantum spin liquid for arbitrary ratio of Γ/K for ferromagnetic Kitaev interaction probably exists [5]. Motivated by the above works, we study the ground-state phase diagram of the extended K-Γ model whose lattice connects the honeycomb lattice, isolated dimers and spin chains. The Hamiltonian is written as,

$$\begin{aligned}\mathcal{H} =&(1-2\lambda)\sum_{\langle ij\rangle_z}\left(-\cos\phi S_i^z S_j^z+\sin\phi(S_i^x S_j^y+S_i^y S_j^x)\right)\\&+\lambda\sum_{\langle ij\rangle_x}\left(-\cos\phi S_i^x S_j^x+\sin\phi(S_i^y S_j^z+S_i^z S_j^y)\right)\\&+\lambda\sum_{\langle ij\rangle_y}\left(-\cos\phi S_i^y S_j^y+\sin\phi(S_i^x S_j^z+S_i^z S_j^x)\right),\end{aligned}$$

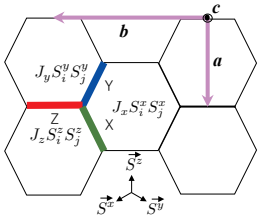

Fig.1 Honeycomb lattice and the Kitaev interaction

where λ is the parameter for the anisotropy. At λ = 1/2, the model describes a spin chain that includes only the *x*- and *y*- bond interactions. At λ =1/3 the interactions become isotropic (honeycomb-lattice), and at λ = 0 the system is equivalent to the isolated dimer model. From the numerical exact diagonalization, we find that there are at least five kinds of phases. Interestingly, one of the five phases is continually connected with the Tomonaga-Luttinger liquid phase at λ = 1/2. This phase and the dimerized phase adjoin each other at λ = 1/3 in a wide range of ϕ.

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Superconducting fluctuations in $S = 1$ one-dimensional Kondo lattice model under transverse magnetic fields

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We study superconducting fluctuations in the $S = 1$ one-dimensional Kondo lattice model (spin-1 KLM) under transverse magnetic fields. Previously, we have studied the effects of the transverse magnetic fields on the spin-1 KLM [1], keeping URhGe in mind. URhGe shows superconductivity inside its ferromagnetic (FM) state and superconducting (SC) transition temperature is strongly enhanced by transverse magnetic fields around $H \sim 12$ T [2]. We have found various phases such as FM phases, Kondo plateau phases, and Tomonaga–Luttinger liquids (TLL) in the ground state of the spin-1 KLM.

In this study, we clarify the relation between SC fluctuations and the transverse magnetic fields h by analyzing SC correlation functions, using the density matrix renormalization group [3]. Since Cooper pairs couple to the $S = 1$ local spins, all the possible SC correlations within the nearest neighbors are taken into account. For example, local pair correlation functions are given by

$$\chi^{\alpha,\beta,\gamma,\delta}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}(r) = \langle \Delta^{\dagger\alpha,\beta}_{\sigma_1,\sigma_2}(N/2)\Delta^{\gamma,\delta}_{\sigma_3,\sigma_4}(N/2+r)\rangle \ , \ \Delta^{\alpha,\beta}_{\sigma_1,\sigma_2}(r) = S^{\alpha}_{r} c_{\sigma_1 r} S^{\beta}_{r} c_{\sigma_2 r}.$$

Here, $c_{\sigma_1 r}$ is the annihilation operator of the conduction electron with spin σ_1 at r site, S^{α}_{r} is the α-component of the $S = 1$ local spin, and N is the system size. The maximum eigenvalue $\chi(r)$ for $\chi^{\alpha,\beta,\gamma,\delta}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}(r)$ corresponds to the leading SC fluctuations. We find that $\chi(r)$ shows a power-law decay $\sim r^{-\theta}$ and the SC fluctuations are enhanced in the TLL phases as shown in Fig. 1.

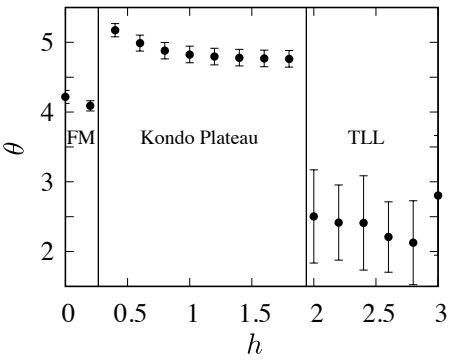

Fig. 1: h dependence of θ, where θ is defined by $\chi(r) \sim r^{-\theta}$.

We will also discuss the nearest-neighbor SC correlations and the effects of transverse magnetic fields on the $S = 1/2$ one-dimensional Kondo lattice model with Ising-type interaction between the local spins.

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Ab initio derivation of effective Hamiltonian for $La_2CuO_4/La_{1.55}Sr_{0.45}CuO_4$ heterostructures

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Superconductivity at interfaces is one of the hottest research topics, where interface atomic layers often show properties superior to the bulk in terms of the critical temperature and its stability [1,2]. One of the most successful examples is the interface between the overdoped $La_{2-x}Sr_xCuO_4$ and Mott insulating La_2CuO_4, where the pinning of T_c at 40 K, which is the optimum T_c of the bulk, was observed in a wide range of $0.2 < x < 0.5$ [2]. Previous variational Monte Carlo study based on the single-band Hubbard Hamiltonian attributed the pinning to the interlayer phase separation [3], but the layer dependence of the effective Hamiltonian was considered only through the difference of the onsite energy level adjusted empirically.

To develop more robust and quantitative understandings of the superconductivity at the LCO/LSCO interface, we have recently derived the layer-dependent two-band (E_g) Hamiltonian by performing large-scale constrained RPA calculations of the $La_2CuO_4/La_{1.55}Sr_{0.45}CuO_4$ superlattice [4]. We have found that the parameters of the superlattice differ considerably from those for the bulk La_2CuO_4, particularly significant in the partially-screened Coulomb parameters and the level offset between the $d_{x^2-y^2}$ and d_{z^2} orbitals. In addition, we have investigated the effect of the lattice relaxation on the E_g Hamiltonian by carefully comparing the parameters derived before and after the structure optimization. We then found that the CuO_6 octahedra distort after the relaxation as a consequence of the Madelung potential difference between the insulator and metal sides, by which the layer dependence of the hopping and Coulomb parameters becomes more gradual than the unrelaxed case. We will discuss the mechanism of the gradual layer dependence of the parameters realized by the lattice relaxation and its potential impact in the superconductivity at the interface.

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Field-Angle Dependence of Interlayer Magnetoresistance in Organic Dirac Electron System

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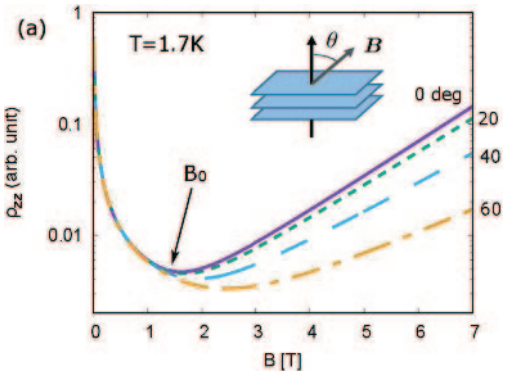
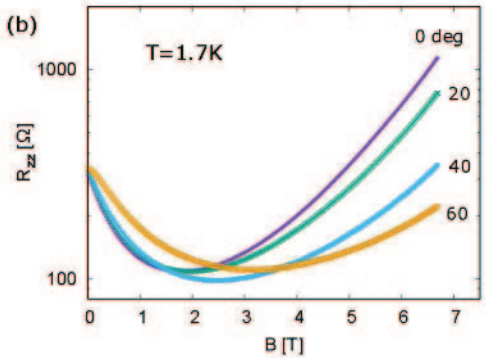
Nowadays, 2-D organic conductor, α-$(BEDT\text{-}TTF)_2I_3$ (α-ET), has attracted much attention because α-ET has the massless Dirac fermions under high pressures. The massless Dirac fermions have many interesting properties, especially in a perpendicular magnetic field. It is known that the N=0 Landau level with the spin splitting emerges at the Dirac point which coincides with the Fermi energy in α-ET. This effect has been detected in interlayer magnetoresistance [1] and the spin lattice relaxation rate [2].

In the present study, we revealed the mechanism of the anomalous field-angle dependence of the interlayer magnetoresistance with a combination of theory and experiment. The enhancement of the effective g-factor obtained in this work is consistent with the results of the Nernst effect [3, 4] and the spin lattice relaxation rate [2].



(a) The theoretical results on B-dependence of ρ_{zz}.



(b) The experimental results on B-dependence of R_{zz}.

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Characterization of quantum chaos by two-point correlators

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Two criteria are widely used currently to characterize quantum chaos: the random-matrix-like universality of the fine-grained energy spectrum and the exponential Lyapunov growth of an out-of-time-order correlation function (OTOC). The Sachdev-Ye-Kitaev (SYK) model, a model of N fermions with all-to-all random interactions, is solvable in the large-N limit and offers a possibility to study a maximally chaotic quantum system. However, the numerical study of the SYK model is limited to small values of N and it remains challenging to observe the exponential growth of OTOC. We have previously generalized the growth exponent of the OTOC to define a spectrum of quantum Lyapunov exponents, which exhibits random matrix behavior when the system is chaotic. [1]

In this work, [2] we propose a simple characterization of quantum many-body chaos. We consider a collection of simple operators and the set of all possible two-point correlation functions, in real time or in imaginary time, between these operators can be organized into a matrix.

We find that the spectral statistics of the singular values of this matrix exhibits universal features characteristic of a random matrix, if the system is in a quantum chaotic phase. We demonstrate this by numerically studying models including the SYK model and a one-dimensional spin chain with random magnetic field. When these models are brought outside the chaotic regime, the spectral statistics significantly deviate from those of known random matrix ensembles and approach those of an uncorrelated distribution. We expect that this correspondence of the behavior of the singular value spectrum of the correlators to the phase of the system can be extended to various types of phase transitions in condensed matter physics.

This work has been done in collaboration with Hrant Gharibyan (Stanford), Masanori Hanada (Southampton), and Brian Swingle (Maryland).

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Canceled

Spin freezing crossover and SYK strange metal

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Multiorbital systems offer a playground of strong correlation physics, including orbital-selective Mott transitions, non-Fermi liquids, and unconventional superconductivity. Those physics can be successfully described by the multiorbital Hubbard model, which finds various material applications such as Sr_2RuO_4 and iron-based superconductors. In the multiorbital Hubbard model with Hund's coupling, there is a competition between the Kondo effect (screening of local magnetic moments) and the Hund effect (formation of local moments), between which emerges a highly moment-fluctuating regime called the spin freezing crossover (Fig. 1). The spin freezing crossover regime shows the anomalous frequency dependence of the self-energy ($\Sigma(\omega)\sim\omega^{1/2}$) and slow relaxation of the spin correlation ($\langle S_z(\tau)S_z(0)\rangle \sim \tau^{-1}$).

Recently, it has been pointed out that such a spin freezing crossover state has a striking similarity to the Sachdev-Ye-Kitaev (SYK) model [1], which shows a maximally chaotic behavior as probed by out-of-time-ordered correlators (OTOCs), and is expected to be a holographic dual to black holes. Motivated by this observation, we study OTOCs for the Hubbard model with a new technique using an imaginary-time four-point function with unusual time ordering [2]. The results show that in the spin freezing crossover regime a spin-related OTOC rapidly decays without oscillations in a short time, and relaxes more slowly as a power law in a long time. This is in a good agreement with the behavior of OTOCs in the SYK model, providing a firm evidence that the spin freezing crossover regime in the multiorbital Hubbard model effectively realizes the SYK strange metal state.

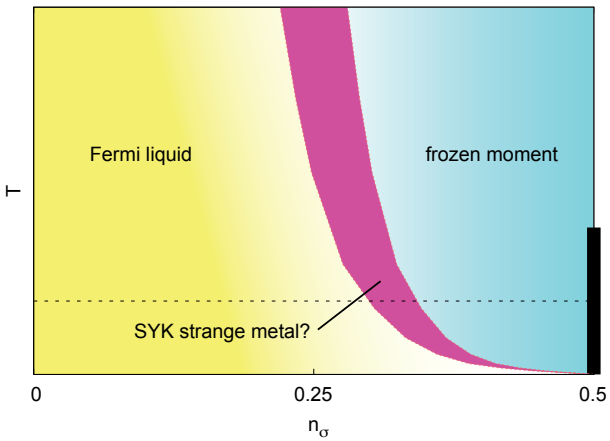

Fig. 1: A schematic phase diagram of the multi-orbital Hubbard model with Hund's coupling.

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Dynamics of fractional excitations in quantum spin ice

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Fractional excitation is one of the surprising manifestations of topologically ordered systems. As a typical example, quantum spin ice, which is known as U(1) quantum spin liquid, hosts fractional excitations, called magnetic monopoles. The monopole excitations draw considerable attention due to their possible roles in the dynamical and transport properties of several candidate materials of quantum spin ice [1]. However, due to the fractional nature of excitations, magnetic monopoles show quite different behaviors from conventional particles, such as magnons, and their character still remains quite elusive.

To understand the nature of magnetic monopoles, we adopt the spin-1/2 XXZ model defined on a pyrochlore lattice. We focus on the region where quantum fluctuation is sufficiently small, and treat the transverse exchange in the first-order degenerate perturbation theory, and obtain the dynamical spectrum of fractional excitations with exact diagonalization (ED) of 32 site cluster. We further construct a hopping model of monopoles by mapping to the three-leaf Husimi cactus, and found that this effective model reproduces the numerical result of ED quite well. The obtained spectrum shows a steep edge at low energy as shown in Fig. 1, which is attributed to van Hove singularity of monopole spectrum, enhanced by the coupling to background “gauge field" [2]. We will discuss the relevance of this result to an actual material, such as $Pr_2Zr(Sn, Hf)_2O_7$, and propose an experiment to identify the U(1) quantum spin liquid, through the observation of fractional excitations.

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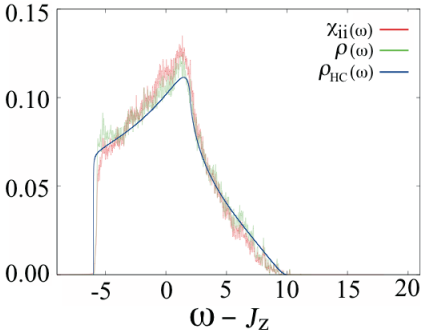

Fig. 1: Two-monopole density of states with ED and the effective model

Topological phase transitions induced by pressure, band-filling, and magnetic field in strongly-correlated pyrochlore iridates

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Recent widespread research in the field of topological quantum states has been exploring the potential role of strong electron correlation which can open a wide range of possible realizations of emergent topological phases. Pyrochlore iridate $R_2Ir_2O_7$ (R=rare-earth ions) is one of the most promising candidates. The forte of this system is that the metal-insulator transition (MIT) can be finely tuned by changing R ions via the modulation bandwidth; the R=Pr compound is paramagnetic metal down to the lowest temperature, while others with smaller R-ionic radius thermally turn into an insulator concomitantly with or separately from the antiferromagnetic (all-in all-out) order at low temperatures [1], reminiscent of a Mott transition system such as vanadates and nickelates. Recent intensive study unveils that the ground state of the R=Pr compound is so-called Luttinger semimetal where a quadratic band touching point exists at the center of Brillouin zone as guaranteed by the lattice symmetry [2]. Interestingly, a symmetry breaking is suggested to turn this state into versatile emergent states including magnetic Weyl semimetal and topological Mott insulator, which remains to be studied.

Here we present several results regarding phase transitions in pyrochlore iridates, which are induced by pressure, band-filling, and magnetic field. (i) Magnetic-field induced MIT is observed in $(Nd,Pr)_2Ir_2O_7$ by electric transport measurements. We suggest that multiple topological electronic states show up near the quantum critical point via modulations of magnetic structures. (ii) A sizable spontaneous Hall effect is accompanied by a vanishingly small magnetization only within the narrow temperature window in the band-width controlled $(Nd,Pr)_2Ir_2O_7$. This is attributable to the emergence of Weyl points in the course of the MIT. (iii) The hole-doping (substitution of R ions with Ca ones) drives the transition from antiferromagnetic insulator to paramagnetic metal in $(Eu,Ca)_2Ir_2O_7$. The thermopower reaches a remarkable value in a wide range of doping level and shows the unique temperature dependence. Combined with the LDA+DMFT calculation, we suggest that the quadratic band touching is a common and robust feature in the paramagnetic metallic phase of hole-doped pyrochlore iridates even in proximity of the Mott transition.

This work is performed in collaboration with Y. Tokura, J. Fujioka, R. Kaneko, N. Nagaosa, R. Arita, B.-J. Yang, and H. Ishizuka.

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Disorder-enhanced quantum fluctuations in a quasi-two-dimensional organic Mott system

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The layered organic conductor κ-$(ET)_2Cu[N(CN)_2]Cl$ (abbreviated to κ-Cl) is an antiferromagnetic (AFM) Mott insulator at ambient pressure, and it exhibits a pressure-induced first-order Mott transition [1,2]. Recent studies of κ-Cl have shown that X-ray irradiation causes drastic changes of charge transport [3] and magnetic properties [4], casting new light on the interplay between electron correlation and disorder.

In the present work, we have performed the transport measurements of a successively X-ray irradiated κ-Cl crystal under continuously controlled He-gas pressure. The most noticeable irradiation effect is the suppression of the Mott critical endpoint, which decreases much more rapidly than the transition temperature of the disorder-sensitive non-s-wave superconductivity, indicating that the Mott critical endpoint is fragile to disorder. In contrast, the quantum critical scaling of resistivity observed in the pristine κ-Cl [5] holds with a similar critical exponent $z\nu$ after the irradiation of 70 hours. The invariant value of $z\nu$ indicates that the system is still in the regime of interaction-driven metal-insulator transition.

As for the magnetism, the ^{1}H NMR measurements revealed the extreme fragility of the commensurate AFM order; it collapses into a randomly-frozen spin state even when the disorder is so weak that the mean distance between the disorder centers is several hundred Å. A further increase in disorder reduces the frozen moments, leading to the emergence of a quantum disordered spin state with gapless excitations.

The present results demonstrate that disorder enhances quantum fluctuations in both the charge and spin degrees of freedom in a quasi-two-dimensional Mott transition system.

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High-throughput search for rare-earth-free permanent magnets

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High performance permanent magnets, or materials with large uniaxial magnetic anisotropy, are needed for a large number of applications, such as electric motors and generators, wind mills, and many more. At the same time these days most high performance magnets contain rare-earth (RE) materials which makes them expensive, while some of the RE elements (like Dy) are rapidly decreasing in availability. According to the assessment of European Union in 2014 not only the RE elements, but also Pt and Co, and phase stabilizers like Ge and In, used in permanent magnets, have been classified as critical raw materials.

Going through a large number of known structures (ICSD database [1]) and using a full-potential linear muffin-tin method with relativistic formulation in RSPt electron structure code [2] to calculate magnetic anisotropy and Curie temperature, we are looking for the materials with high magnetization >1 T, uniaxial anisotropy >1 MJ/m^3, and T_c>300 K to identify the suitable replacement for hazardous materials, without a loss of performance in permanent magnets.

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Thermoelectric effects in a doped spin liquid candidate κ-$(ET)_4Hg_{2.89}Br_8$

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κ-$(ET)_4Hg_{2.89}Br_8$ is a quasi-two-dimensional organic conductor that possibly host a doped spin liquid [1]. The previous studies revealed a pressure-induced crossover or transition from a non-Fermi liquid (NFL) to a Fermi liquid (FL) in resistivity behavior (Fig.1) and from a low to high carrier-density states in the Hall coefficient [2]. The superconductivity that emerges at low temperatures was suggested to exhibit a crossover from local to extended paring with increasing pressure by the evaluation of the coherence length [3]. These results imply that a crossover from NFL/BEC to FL/BCS is driven by the change of electron correlation.

In the present work, we investigated thermoelectric effects, which are useful to reveal the electronic states, for κ-$(ET)_4Hg_{2.89}Br_8$ under pressure. We found that, in the crossover pressure region, the Seebeck coefficient divided by temperature, S/T, are enhanced at low temperatures (Fig.2) and its temperature dependence is logarithmic. Similar logarithmic enhancement of S/T is also reported in other systems situated in the vicinity of quantum phase transitions, suggesting that the present observation originates from NFL-FL quantum critical fluctuations. Regarding the superconductivity, the Nernst voltage is generated at higher temperature than T_c and keeps large values at higher magnetic fields in the low-pressure regime than in the high-pressure regime, indicating that superconducting fluctuations are strongly enhanced in the doped spin liquid state at low pressures.

The present results of thermoelectric studies support a quantum phase transition or crossover between a correlated metal and a doped spin liquid, followed by a BEC-BCS crossover at low temperatures.

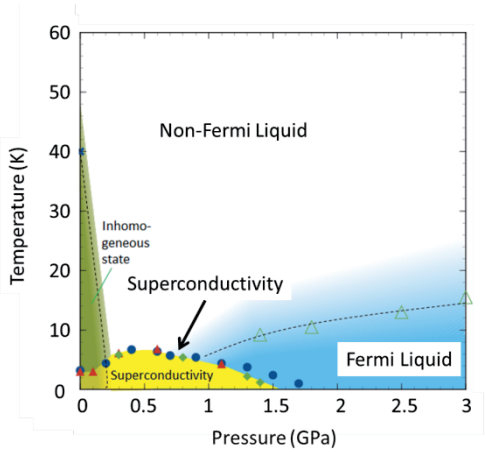

Fig. 1: Phase diagram of κ-HgBr [4]

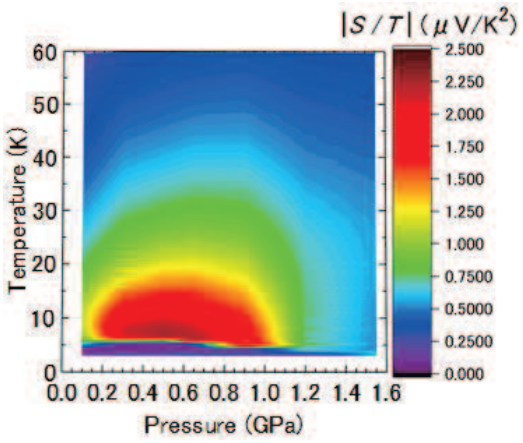

Fig. 2: Color plot of $|S/T|$ in κ-HgBr

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Two Competing Superconducting Phases in Molecular Conductors κ-(BEDT-TTF)$_2$X

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Unconventional superconductivity (SC) is often observed around the Mott transition in strongly-correlated electron system. In the family of molecular conductors κ-(BEDT-TTF)$_2$X with a 3/4-filled energy band, the application of external pressure or chemical substitution of X to the so-called dimer-Mott insulators induces SC whose gap symmetry is still controversial [1]. Although κ-(BEDT-TTF)$_2$X is often compared with the high-T_c cuprates with several similarities [2], there are also differences which should be carefully examined. In κ-(BEDT-TTF)$_2$X, SC appears next to the nonmagnetic Mott insulators as well as the AF Mott insulators. It is not clear whether the AF spin fluctuation mechanism discussed in the cuprates can be directly applied to κ-(BEDT-TTF)$_2$X. Furthermore, the intradimer charge degree of freedom, which is a character of molecular materials, plays important roles as suggested in the anomalous dielectric responses and Raman spectroscopies.

In this study, we investigate the extended Hubbard model for κ-(BEDT-TTF)$_2$X where the intradimer charge degree of freedom and the intersite (long-range) Coulomb interactions are explicitly considered. The variational Monte Carlo method is used for the analysis of the ground-state properties. We obtain the ground-state phase diagram for both bandwidth-control [3] and filling-control [4] cases. There appear various competing phases: dimer-type AF phase, polar charge-ordered phase, two 3-fold charge-ordered phases, and two SC phases with different gap symmetries. The "extended-s+$d_{x^2-y^2}$"-wave SC is favored for the electron-doped side and the "d_{xy}"-wave SC, which is similar to the symmetry in the cuprates, is favored for the hole-doped side. We show the origin of two SC phases from the viewpoint of spin/charge fluctuations and the geometrical frustration unique to κ-(BEDT-TTF)$_2$X.

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Theory of Proton-Driven Quantum Spin-Dipole Liquids

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We present a theory of a hybrid quantum liquid state, quantum spin-dipole liquid (QSDL), in a hydrogen-bonded electron system, by combining the concepts of a quantum proton ice and Anderson's resonating valence bond (RVB) theory [1], motivated by the recent experimental discovery of a proton-driven QSDL in κ-H_3(Cat-EDT-TTF)$_2$ called H-Cat [2]. In this material, it was observed experimentally that quantum spin liquid is strongly coupled to quantum proton motion. In our theory, an electron spin liquid and a proton dipole liquid are realized simultaneously, while none of them can be established independently. Analytical and numerical evaluations of entanglement entropy reveal that this state is far beyond the crude Born-Oppenheimer approximation, showing a volume-law entanglement entropy between spins and dipoles. We also examine the stability of QSDL against perturbations and discuss implications for the experiments in H-Cat and its deuterated analog D-Cat.

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Phase transitions in non-Hermitian fermionic superfluidity under complex-valued interactions

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In recent years, non-Hermitian (NH) quantum systems have been actively studied both experimentally and theoretically. It has been revealed that non-Hermiticity drastically alters the properties of a number of quantum phenomena that have been established in the Hermitian physics [1,2]. Such theoretical predictions have been confirmed experimentally by using optical systems and ultracold atoms. However, since most of the previous studies dealt with single-particle physics, understanding of many-body physics in NH systems is yet in its infancy.

Motivated by recent experimental advances in ultracold fermionic atoms, we analyze a non-Hermitian (NH) BCS Hamiltonian with complex-valued interactions arising from inelastic scattering between fermions. We develop a mean-field theory to obtain a NH gap equation for order parameters, which are similar to but different from the standard BCS ones because of the inequivalence of left and right eigenstates in the NH physics. We find unconventional phase transitions unique to NH systems: the superfluidity breaks down and reappears with increasing dissipation, featuring non-diagonalizable (exceptional) points, lines, and surfaces in the quasiparticle Hamiltonian for weak attractive interactions. As for strong attractive interactions, the superfluid gap never collapses but is enhanced by dissipation due to an interplay between the BCS-BEC crossover and the quantum Zeno effect. Our results lay the groundwork for studies of fermionic superfluidity of ultracold atoms under inelastic collisions.

Acknowledgement: This work is done in collaboration with Masaya Nakagawa (RIKEN), Kazuaki Takasan (Kyoto Univ.), Kyosuke Adachi (Kyoto Univ.), Masahito Ueda (Univ. of Tokyo &RIKEN).

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Non-Hermitian perspective of strongly correlated systems

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Norio Kawakami[2], and Yasuhiro Hatsugai[1]

[1] University of Tsukuba, [2] Kyoto University

Recently, a variety of new topological phenomena have been reported for non-Hermitian systems. So far, such phenomena are supposed to be observed for non-equilibrium systems. Interestingly, however, it became clear that non-Hermitian phenomena may emerge even in equilibrium systems because of finite lifetime of quasi-particles. The analysis based on the perturbation theory elucidates the emergence of exceptional points accompanied by bulk Fermi arcs [1].

Inspired by the above results, we analyze strongly correlated systems where the effects of quasi-particle damping are important. Specifically, we address the following two issues.

(i) Numerical observation of the exceptional points beyond the perturbation theory [2].

We address this issue by analyzing the heavy-fermion systems with DMFT+NRG. In addition to the emergence of exceptional points we observe that the lattice periodicity results in the fusion of exceptional points and the bulk Fermi loop.

(ii) Interplay of symmetry and exceptional points: emergence of symmetry-protected exceptional rings and torus [3].

In the second part, we analyze the interplay of exceptional points and symmetry which plays an important role for Hermitian topological systems. We analyze the systems with chiral symmetry as an example and observe that the symmetry-protection results in novel topological degeneracies which we call symmetry-protected exceptional rings and torus. The former and the latter are observed for two and three dimensions, respectively. In addition, we propose a honeycomb lattice model hosting the above topological degeneracies.

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Constructing Neural Stationary States for open quantum many-body systems

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The dramatic development of machine learning techniques has inspired physicists to invent new numerical algorithms that further explore the frontier of condensed matter physics. Successful applications include the phase classification using the well-established algorithms such as the deep learning [1,2] and the representation of the quantum many-body states using the high expressive power of the neural networks [3].

Despite its rapid progress, however, machine-learning-based algorithms have yet to be applied to one of the most challenging problems in modern physics -- open quantum many-body systems. Due to the growth of the number of parameters in proportion to the square of the Hilbert space dimension, description of the quantum states by density matrices requires additional computational resource compared to the closed system.

In this work, we present a new scheme for simulating the stationary states of open quantum many-body systems by employing the ansatz based on the neural-network quantum states [4]. See Fig.1 for a schematic illustration of our method. Using the high expressive power of the variational ansatz described by the restricted Boltzmann machines (RBM), the stationary states of the Lindblad dynamics is computed. After mapping the stationary-state search problem into finding a zero-energy ground state of an appropriate Hermitian operator, we apply the conventional variational Monte Carlo method for optimization. Our method is shown to simulate various spins systems efficiently, i.e., the transverse-field Ising models in both one and two dimensions and the XYZ model in one dimension.

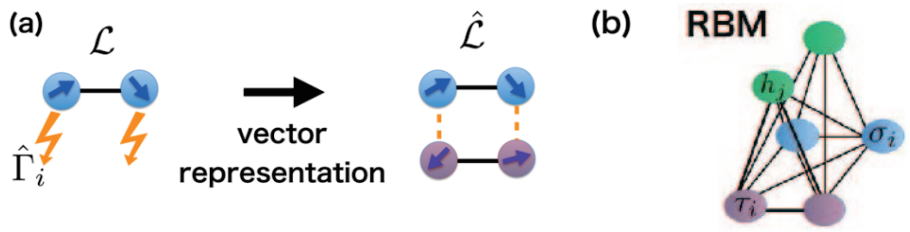

Fig. 1: Schematic illustration of our method for the case with two spins.
(a) (Left) A spin model with dissipations. (Right) The vector representation of the Lindbladian as on the doubled Hilbert space.
(b) Neural stationary state represented by the RBM, which is composed of the physical spins σ_i, fictitious spins τ_i, and hidden spins h_j.

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