PROGRAM AND ABSTRACTS

Computational Quantum Many-Body Theory

July 17 – 19, 2024

Rm. 1503, KIAS, Seoul

Plenary Speakers

Jan von Delft, LMU Munich, Germany

Philipp Werner, University of Fribourg, Switzerland

Ryotaro Arita, University of Tokyo, Japan

Invited Speakers

Chang-Yeon Moon, KRISS, South Korea

Fabian Kugler, Flatiron Institute, USA

Gil Young Cho, Postech, South Korea

Heung-Sik Kim, Kangwon National Univ., South Korea

Hong Chul Choi, MPK-Postech, South Korea

Hongkee Yoon, Kangwon National Univ., South Korea

Ji Hoon Shim, Postech, South Korea

Kun Chen, ITP-CAS, China

Kyusung Hwang, KIAS, South Korea

Moon Jip Park, Hanyang University, South Korea

Myung Joon Han, KAIST, South Korea

Nicola Lanata, Rochester Institute of Technology, USA

Wei Li, ITP-CAS, China

Yusuke Nomura, Tohoku University, Japan

Session Chairs

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Bongjae Kim, Kyungpook National University, South Korea

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Se Young Park, Soongsil University, South Korea

	July 17 (Wed)	July 18 (Thu)	July 19 (Fri)
9:00-9:30	Registration		
9:30-10:30	Chair: Hyoung Joon Choi	Chair: Seunghoon Lee	Chair: Bongjae Kim
	Ryotaro Arita	Jan von Delft	Philipp Werner
10:30-11:10	Ji Hoon Shim	Fabian Kugler	Hongkee Yoon
11:10-11:50	Myung Joon Han	Kun Chen	Gil Young Cho
11:50-13:30	Lunch		
13:30-14:10	Chair: Ara Go	Excursion and Dinner	Chair: Hyun-Yong Lee
	Kyusung Hwang		Moon Jip Park
14:10-14:50	Hong Chul Choi		Nicola Lanata
14:50-15:20	Coffee Break		Coffee Break
15:20-16:00	Chair: Geunsik Lee		Chair: Chang-Jong Kang
	Chang-Yeon Moon		Yusuke Nomura
16:00-16:40	Wei Li		Heung-Sik Kim
16:40-17:20	Poster Session		
17:20-18:00			
18:00	Dinner		

ABSTRACTS OF TALKS

Coherence length and penetration depth in strongly correlated multi-orbital superconductors

Ryotaro Arita

Research Center for Advanced Science and Technology, University of Tokyo
RIKEN Center for Emergent Matter Science

The penetration depth and coherence length are the most fundamental parameters describing the superconducting state, alongside the transition temperature. Once these quantities are determined, the critical current and critical magnetic field can be calculated, allowing the determination of the phase diagram of the superconducting state. In this talk, we will discuss the calculation of the penetration depth and coherence length in multi-orbital strongly correlated electron systems, taking C_{60} superconductors as an example.

Alkali-doped C_{60} superconductors are known as the systems with the highest transition temperatures among molecular solids. While the unit cell contains 63 atoms, the low-energy electronic states near the Fermi level are described by a simple three-orbital model based on the t_{1u} molecular orbitals [1], and their superconducting mechanism can be precisely calculated using the dynamical mean field theory (DMFT).

In this talk, it will first be shown that this system can be effectively represented by a multi-orbital model with an effective negative Hund's coupling as a result of strong electron-lattice interactions. By determining the parameters in this three-orbital model from first principles and calculating the superconducting transition temperature as a function of the lattice constant of the system, we obtain results that quantitatively agree well with experimental data [2].

Next, we will show the results of the DMFT calculation of the coherence length and penetration depth. The calculated values are well aligned with experimental results. We observe that increasing the values of Hubbard U and Hund's coupling J decreases the coherence length, shifting the superconducting state from BCS-like to BEC-like. Interestingly, increasing U suppresses the transition temperature towards a BEC-like state, whereas increasing J does not show such suppression, which is unusual in correlated electron systems [3].

[1] Y. Nomura, K. Nakamura, R. Arita, Phys. Rev. B 85, 155452 (2012)
[2] Y. Nomura, *et al*., Science Advances, 1 e1500568 (2015)
[3] N. Witt, *et al*., arXiv:2310.09063

Low Energy Effectiveness induced by Hund Correlation

Dongwook Kim[1], Ina Park[1], Bo Gyu Jang and Ji Hoon Shim[1,*]

[1]*Department of Chemistry, Pohang University of Science and Technology, Pohang 37673, Republic of Korea*

Strong correlation from Hund interaction has vastly studied among the decade. Various peculiar phenomena were discovered both experimentally and theoretically, where the only-Hubbard correlated systems couldn't sh. One of the successes was the discovery of Hund metal where the Hubbard correlation was small in contrast to large Hund correlation, leading to low coherence scale in contrast to the difficulty to the metal-insulator transition (MIT). However, not many studies have focused on how the Hund correlation influences on the behavior during the evolution toward the Mott insulator. Recently studies on $NiS_{2-x}Se_x$ have focused on the Hund physics and its role on Brinkman-Rice (BR) violation due to the low-energy effectiveness (LEE) of the bandwidth renormalization, showing strong bandwidth renormalization only on low-frequency scale, i.e. kink scale. In this study, we have quantified the LEE of Hund correlation by defining the correlation factors at low- and high- energy scales which describe the correlation strength at each energy scale. The evolution of the correlation factors during the MIT, which can be corresponded to the evolution of the peak width at the Fermi level and the reduction of overall conduction band, illustrated clear BR violation originating from the LEE of Hund correlation. The origin of LEE has explained by its equivalence to the spin-degree-of-freedom effectiveness (SDFE), which is observed from the evolution of spin and charge susceptibilities.

Recent Progress of 'Jx' code for magnetic force linear response theory and its applications

Myung Joon Han

Department of Physics, KAIST

In this talk, I will report our recent progress of 'Jx' code [1, 2] for calculating magnetic interactions in molecules and solids based on magnetic force theorem (MFT). Originally started from a 'OpenMX' subroutine [3, 4], 'Jx' has been separated and re-written in Julia to foster more active developments. In the first part of this presentation, I will try to introduce the basic idea of MFT formalism with a particular emphasis on the less-known features [5]. 'Jx' has been successfully combined with more advanced schemes of self-energy computations including QSGW (quasi-particle self-consistent GW) [6] and single-site DMFT (dynamical mean-field theory) [7]. For the former, this implementation can be particularly useful because the total energy is typically not accessible. Last couple of years efforts have focused on the spin-orbit coupled case whose Hamiltonian includes such terms as Dzyaloshinskii-Moriya and Kitaev-Gamma [8]. After a brief introduction to this extended formalism, I will present some results of real material examples.

[1] H. Yoon, T. J. Kim, J. -H. Sim, M. J. Han, Comp. Phys. Comm. 247, 106927 (2020).
[2] https://kaist-elst.github.io/Jx.jl/
[3] M. J. Han, T. Ozaki and J. Yu, Phys. Rev. B 70, 184421 (2004).
[4] https://openmx-square.org/
[5] H. Yoon, T. J. Kim, J. -H. Sim, S. W. Jang, T. Ozaki, M. J. Han, Phys. Rev. B 97, 125132 (2018).
[6] H. Yoon, S. W. Jang, J. -H. Sim, T. Kotani, M. J. Han, J. Phys.: Condens. Matter 31 405503 (2019).
[7] H. J. Lee et al., (in preparation)
[8] D. H. Kiem et al., (in preparation)

The Ghost Gutzwiller Approximation: Recent algorithmic advancements and applications

Nicola Lanatà

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Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA

The Ghost Gutzwiller Approximation (gGA), a computationally efficient extension of the multi-orbital Gutzwiller Approximation, has demonstrated substantial accuracy in simulating the quantum-mechanical properties of strongly correlated materials, comparable to the Dynamical Mean-Field Theory (DMFT) while significantly reducing computational demands. This talk presents the latest advancements in the gGA framework, emphasizing the integration of machine learning techniques to further diminish the computational overhead. We detail how these innovations allow for more rapid and accurate simulations, thereby accelerating the exploration of complex material systems. Additionally, we discuss recent benchmark results that highlight the enhanced performance and reliability of gGA in various strongly correlated scenarios.

DFT+DMFT studies on f-electron systems: correlation, universality, and topology

Hongchul Choi

Max Planck POSTECH Korea Research Initiative, Pohang, 37673, Korea

In Cerium-based heavy electron materials, the 4f electron's magnetic moments bind to the itinerant quasiparticles to form composite heavy quasiparticles at low temperature. The volume enclosed by the Fermi surface (FS) in the Brillouin zone incorporates the moments so that a large FS occurs with correlation effect. On the other hand, when the f electrons are localized free moments, the FS contains only conduction spd electrons, resulting in a small FS. So, the FS volume is a sensitive probe of the heavy fermion system's nature, whether 4f electrons are localized or itinerant. The combination technique of density function theory and dynamical mean field theory (DFT+DMFT) computation enables us to understand this crossover in Ce-based heavy fermion systems in between a small FS and a large FS in terms of two characteristic temperatures [1,2]. Furthermore, we explored how electron or hole doping alters the nature of 4f electrons [3]. Recently, the effect of the crystalline electric field on the Ce-based heavy fermion system was revisited, showing its importance at very low temperature to determine a ground state below two characteristic temperatures [4]. If time permits, we will address the potential platform that f-electron systems could provide to realize the topological correlation systems [5,6].

[1]HCC, B. I. Min, J. H. Shim, K. Haule, and G. Kotliar, Phys. Rev. Lett. 108, 016402 (2012).
[2]HCC, K. Haule, G. Kotliar, B. I. Min, and J. H. Shim, Phys. Rev. B 88, 125111 (2013).
[3] HCC, Eric D Bauer, Filip Ronning, Jian-Xin Zhu, Phys. Rev. B 105, 115121 (2022).
[4] Bo Gyu Jang, Beomjoon Goh, Junwon Kim, Jae Nyeong Kim, Hanhim Kang, Kristjan Haule, Gabriel Kotliar, HCC, Ji Hoon Shim, Phys. Rev. B 105, 115147 (2022).
[5]HCC et al. "Experimental and theoretical study of topology and electronic correlations in PuB4" Phys. Rev. B 97, 201114 (2018).
[6]Ryu, Dong-Choon, et al. "Wallpaper Dirac Fermion in a nonsymmorphic topological kondo insulator: PuB4." *Journal of the American Chemical Society* 142, 19278 45 (2020)

Symmetry of superconducting order parameters in Sr_2RuO_4 from DFT+DMFT

Chang-Youn Moon

Korea Research Institute of Standards and Science

Superconducting gap functions are obtained by solving the linearized Eliashberg equation set up from the spin and charge susceptibilities calculated within DFT+DMFT. First, the impact of frequency dependence of the two-particle vertex, estimated in the CTQMC impurity solver, on the symmetry of the order parameter is discussed. Adopting the dynamic two-particle vertex is found to alter the peak position of the effective repulsive pairing interaction in the momentum space compared with using the conventional static vertex as in random-phase approximation, RPA, leading to nearly degenerate *s*- and *d*- wave gap functions, followed by an odd-orbital/odd-parity gap solution, all in spin-singlet state. Orbital selectivity in this Hund's metal turns out to play an important role here. Next, peculiar gap solutions in the frequency dependent version of the linearized Eliashberg equation are considered. Unusual four-fold degenerate gap solutions are found, where two-fold degeneracy is from the lattice symmetry while the other two-fold degeneracy is from decoupling between frequency/orbital components of the effective pairing potential. Even- and odd-frequency/orbital solutions are degenerate in this case, and the possibility of consequent unusual superconducting properties, such as zero energy gap and time-reversal symmetry breaking, is discussed.

Quantum Supercriticality: Universal Crossover Scalings and Rydberg Atom Simulation

Wei Li

Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China

Supercriticality, featured with universal scaling behaviors, emerges as an intriguing phenomenon proximate to the classical liquid-gas critical point. In this talk, we extend this significant concept to quantum many-body systems near the quantum critical point, employing tensor network calculations and scaling analyses of the Ising model and Rydberg atom array. The supercritical quantum states are found to be strongly fluctuating and highly entangled, as characterized by the universal scalings in susceptibility, correlation length, fidelity susceptibility, and entanglement entropy. The universal scaling behaviors are revealed in the regime enclosed by two quantum supercritical crossover lines in the longitudinal-transverse field plane, where the response functions, measures of entanglement, and fidelity susceptibility reach their maxima. The present work establishes a foundation for exploring quantum supercriticality in magnetic systems and through quantum simulations. Specifically, we suggest that Rydberg atom arrays offer an ideal platform for simulating the “liquid-gas” phase transition in the quantum realm and for investigating the associated universal scaling phenomena, utilizing both conventional response functions and quantum information metrics.

Quantum Criticality and Strange-Metal Behavior – a DMFT+NRG Perspective

Jan von Delft

Ludwig Maximilian University Munich

Strange metals are enigmatic states of matter found in the phase diagrams of a large number of strongly correlated materials, such as cuprate superconductors, iron based superconductors, twisted bilayer graphene, or heavy-fermion metals. They show T-linear resistivity and a $\sim T \ln T$ specific heat, and often ω/T scaling of dynamical susceptibilities and of the optical conductivity.

I will discuss strange-metal behavior found in the quantum-critical region of two paradigmatic models of correlated metals. We obtain access to unprecedentedly low energy scales by using cellular dynamical mean-field theory (CDMFT) with the numerical renormalization group (NRG) as a real-frequency cluster impurity solver.

(i) We used 2-site CDFMT+NRG to study paramagnetic quantum criticality in the periodic Anderson model (PAM), describing itinerant c electrons hybridizing with a lattice of localized f electrons. At zero temperature, it exhibits a quantum phase transition from a Kondo phase to an RKKY phase when the hybridization is decreased through a so-called Kondo breakdown quantum critical point (KB–QCP). There, Kondo screening of f spins by c electrons breaks down, so that f excitations change their character from somewhat itinerant to mainly localized, while c excitations remain itinerant. In the quantum critical region, we find that the staggered spin exhibits SYK-like slow dynamics and its dynamical susceptibility shows ω/T scaling. We propose a scaling Ansatz that describes this behavior. It also implies Planckian dissipation for the longest-lived excitations. The current susceptibility follows the same scaling ansatz, leading to strange-metal scaling. Surprisingly, the SYK-like dynamics and scaling are driven by strong vertex contributions to the susceptibilities. Our ω/T scaling results for the optical conductivity match experimental observations on $YbRh_2Si_2$ and $CeCoIn_5$.

(ii) We used 4-site plaquette DMFT+NRG to study quantum criticality in the 2-dimensional Hubbard model for cuprate superconductors. This model has a QCP as a function of hole doping. In its quantum-critical region we find several indications of strange-metal behavior, including ω/T scaling for the optical conductivity matching experimental observations on $La_{1.76}Sr_{0.24}CuO_4$.

arXiv:2310.12672, arXiv: 2404.14079

Hund Metals in Models and Materials -- a DMFT+NRG Perspective

Fabian Kugler

Center for Computational Quantum Physics, Flatiron Institute, New York, NY, USA

tba

Unveiling the "Lost Coulomb Pseudopotential" in Sub-Kelvin Superconductors

Kun Chen

Institute of Theoretical Physics, Chinese Academy of Science

Sub-Kelvin superconductors are essential for quantum computation and sensitive detectors, but understanding the electron pairing mechanism and correlation effects in these systems remains a challenging frontier. We present a refined theory of quasiparticle pairing in these systems, built on an effective field theory (EFT) approach. To implement this theory, we introduce an innovative AI-powered numerical framework that enables efficient and accurate computation of high-order Feynman diagrams. Our calculations reveal that traditional theories significantly underestimate the strength of the pseudopotential, resolving the long-standing lost Coulomb pseudopotential problem and emphasizing its critical role in these systems. We also propose a universal finite-temperature scaling law for predicting new sub-Kelvin superconductors and identify potential candidates among elemental metals. Our findings provide new insights into exploring novel superconducting materials, understanding sub-Kelvin superconductivity mechanisms, and developing advanced superconducting electronics.

Nonequilibrium dynamical mean field theory

Philipp Werner

University of Fribourg, 1700 Fribourg, Switzerland

The study of nonequilibrium phenomena in correlated electron systems, such as laser-induced switching of solids to metastable hidden phases, is an active research frontier in condensed matter physics. Theoretical studies and simulations of the underlying processes are challenging, and numerical techniques are still under development. A promising approach is the nonequilibrium extension of dynamical mean field theory. After reviewing the formalism and its implementation with currently available nonequilibrium solvers, I will discuss recent applications to nonthermal hidden phases in strongly correlated systems. In particular, I will show that this method allows us to realize nonthermal magnetic, superconducting and excitonic orders, and to map out nonequilibrium phase diagrams of photo-doped Mott insulators.

Scaling Up Atomic Simulations: Machine Learning Potentials and Diffusion Models

Hongkee Yoon[1,2]
[1]*Kangwon National University*
[2]*KIAS Center for Artificial Intelligence and Natural Sciences*

In this talk, we present our recent works on accelerating atomic-scale simulations by developing and applying machine learning potentials and diffusion models. Machine learning has emerged as a powerful tool, enhancing the efficiency of calculations to unprecedented levels. We have addressed the stability issues of machine learning potentials by incorporating regularization techniques and data augmentation strategies, enhancing their robustness and transferability. Furthermore, we introduce a novel transformer-based model that efficiently represents atomic environments, significantly improving these potentials' accuracy and computational efficiency, enabling large-scale simulations that were previously intractable[1-3]. Additionally, we demonstrate our work on diffusion models for generating stable molecular structures by integrating physical ideas and constraints, such as energy-based constraints and symmetry considerations, into the learning process[4]. These advancements in machine learning potentials and diffusion models would provide a framework for accelerating atomic-scale simulations and unlocking new insights into material properties and design.

1. Towards Physically Reliable Molecular Representation Learning. UAI (2023)
2. Molecular Dynamics Study of Silicon Carbide Using an Ab Initio-Based Neural Network Potential: Effect of Composition and Temperature on Crystallization Behavior. J. Phys. Chem. C (2023).
3. Deep-DFT: A Physics-ML Hybrid Approach to Predict Molecular Energy using Transformer. NeurIPS workshop (2021).
4. Hybrid Diffusions for Stable Molecular Structure Generation via Explicit Energy-based Model. (ICML) Workshop, (2023).

Non-Abelian Fractional Quantum Anomalous Hall States and First Landau Level Physics in Second Moiré Band of Twisted Bilayer $MoTe_2$

Gil Young Cho[1,2,3]

[1]*Department of Physics, Pohang University of Science and Technology, Pohang, 37673, Republic of Korea*
[2]*Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science, Pohang 37673, Korea*
[3]*Asia-Pacific Center for Theoretical Physics, Pohang, Gyeongbuk, 37673, Korea*

Utilizing the realistic continuum description of twisted $MoTe_2$ and many-body exact diagonalization calculation, we establish that the second moiré band of twisted $MoTe_2$, at a small twist angle of approximately two degrees, serves as an optimal platform for achieving the long-sought non-Abelian fractional quantum anomalous Hall states without the need for external magnetic fields. Across a wide parameter range, our exact diagonalization calculations reveal that the half-filled second moire band for a broad range of parameters demonstrates the ground state degeneracy, which is consistent with the pfaffian state in the first Landau level. We further elucidate that the emergence of the non-Abelian state is deeply connected to the remarkable similarity between the second moiré band and the first Landau level. Essentially, the band not only exhibits characteristics akin to the first Landau level, but also that its projected Coulomb interaction closely mirrors the Haldane pseudopotentials of the first Landau level. Motivated from this observation, we also introduce a novel metric of "the first Landau level"-ness of a band, which quantitatively measures the alignment of the projected Coulomb interaction with the Haldane pseudopotentials in Landau levels. This metric is then compared with the global phase diagram including the non-Abelian fractional quantum anomalous Hall state, revealing its utility in predicting the parameter region of the non-Abelian state. We finally discuss the potential implications on experiments.

Non-Hermitian many-body physics

Moon Jip Park

Hanyang University, Department of Physics

The presence of gain and loss in open quantum systems open new dimensions in the knowledge of condensed matter physics. The synthesis of non-Hermiticity with many-body interactions introduces unprecedented phenomena such as enhanced state localization, altered phase transitions, and novel topological invariants that are not observable in purely Hermitian systems. Here, I present the recent research in the discovery of non-Hermitian topological phases in the presence of the interactions. We explore the implications of the non-Hermitian skin effect in collective settings, illustrating how these topological phases persist and reshape the conventional understanding of localization and spectral properties.

Mixed-State Quantum Spin Liquids and Dynamical Anyon Condensations in Kitaev Lindbladians

Kyusung Hwang

Korea Institute for Advanced Study

Quantum spin liquids and anyons, used to be subjects of condensed matter physics, now are realized in various platforms of qubits, offering unprecedented opportunities to investigate fundamental physics of many-body quantum entangled states. Qubits are inevitably exposed to environment effects such as decoherence and dissipation, which are believed to be detrimental to many-body entanglement. Here, we argue that unlike the common belief decoherence and dissipation can give rise to novel topological phenomena in quantum spin liquids. We study open quantum systems of the Kitaev spin liquid and the toric code via the Lindblad master equation approach. By using exact solutions and numerical approaches, we show the dynamical occurrence of anyon condensation by decoherence and dissipation, which results in a topological transition from the initial state spin liquid to the steady state spin liquid. The mechanism of the anyon condensation transition by the Lindblad dynamics is elucidated. We also provide an insight into the relationship between the Kitaev spin liquid and the toric code in the picture of anyon condensation. Our work suggests open quantum systems to be a new venue for topological phenomena of quantum spin liquids and anyons.

[Preprint] Hwang, arXiv:2305.09197.

Fermi Surface Expansion above Critical Temperature in a Hund Ferromagnet

Yusuke Nomura

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Understanding the effects of electron correlations beyond Fermi liquid theory is a fundamental problem in condensed matter physics. This is because a variety of interesting phenomena, such as superconductivity and magnetism, arise from strange metallic states.

A well-known example is the pseudogap behavior observed in doped cuprates, where nonlocal antiferromagnetic fluctuations are believed to play a critical role. This phenomenon has been intensively studied by the cluster extension of the dynamical mean-field theory.

However, nonlocal correlation effects in multiorbital systems are largely unexplored. In particular, the influence of ferromagnetic fluctuations in the strong coupling regime is still poorly understood compared to the antiferromagnetic case.

Such a strong coupling ferromagnetic regime is expected in the multiorbital Hubbard model. Therefore, we study the two-orbital Hubbard model on the two-dimensional square lattice using cellular dynamical mean-field theory. Although the cluster extension in multiorbital systems is computationally expensive, we have achieved to accomplish the calculations thanks to the efficient continuous-time quantum Monte Carlo methods developed in Refs. [1-3].

We find that the Fermi surface expands even above the Curie temperature as if the spin polarization occurred, contrary to a naive view that the Fermi surface should behave as a non-spin-polarized state. Behind this phenomenon, effective “Hund’s physics” works in momentum space; ferromagnetic spin correlations induce effective Hund’s coupling in momentum space, leading to a large modulation of the momentum space occupancy. The reconstruction of the Fermi surface differs from the antiferromagnetic case, where it creates hot and cold spots in the Fermi surface. Our finding will give a deeper insight into the physics of Hund’s ferromagnets above the Curie temperature [4,5].

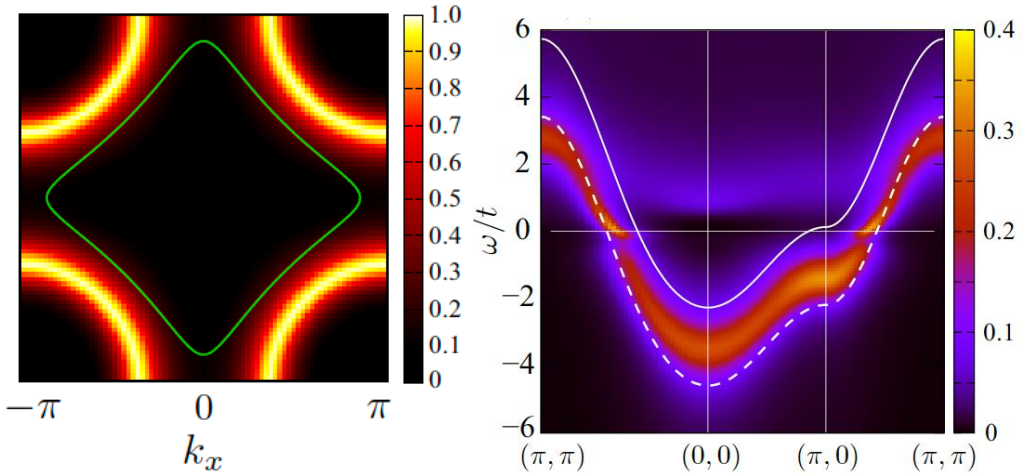

Fig. 1: Fermi surface and spectral function in a Hund ferromagnet above critical temperature.

[1] Y. Nomura, S. Sakai, and R. Arita, Phys. Rev. B **89**, 195146 (2014)

[2] H. Shinaoka, Y. Nomura et al., Phys. Rev. B **92**, 195126 (2015)

[4] H. Shinaoka, Y. Nomura and E. Gull, Comput. Phys. Commun. **252**, 106826 (2020)

[4] Y. Nomura, S. Sakai, and R. Arita, Phys. Rev. B **91**, 235107 (2015)

[5] Y. Nomura, S. Sakai, and R. Arita, Phys. Rev. Lett. **128**, 206401 (2022)

Correlation-induced flat bands and ferromagnetic fluctuations in Mn-based kagome metal

Heung-Sik Kim

Department of Semiconductor Physics, Kangwon National University, Chuncheon 24341, Korea

Kagome lattice has been actively studied for the possible realization of frustration-induced two-dimensional flat bands and a number of correlation-induced phases. Currently, the search for kagome systems with a nearly dispersionless flat band close to the Fermi level is ongoing. Here, by combining theoretical and experimental tools, we present $Sc_3Mn_3Al_7Si_5$ as a novel realization of correlation-induced almost-flat bands in the kagome lattice in the vicinity of the Fermi level. Our magnetic susceptibility, ^{27}Al nuclear magnetic resonance, transport, and optical conductivity measurements provide signatures of a correlated metallic phase with tantalizing ferromagnetic instability. Our dynamical mean-field calculations suggest that such ferromagnetic instability observed originates from the formation of nearly flat dispersions close to the Fermi level, where electron correlations induce strong orbital-selective renormalization and manifestation of the kagome-frustrated bands. In addition, a significant negative magnetoresistance signal is observed, which can be attributed to the suppression of flat-band-induced ferromagnetic fluctuation, which further supports the formation of flat bands in this compound. These findings broaden a new prospect to harness correlated topological phases via multiorbital correlations in 3d-based kagome systems.

ABSTRACTS OF POSTERS

Poster No.1

Dynamical properties of 1D spin models via complex time evolution implemented in DMRG

Jeong Hyeok Cha[1*], Heung-Sik Kim[1] , and Hyun-Yong Lee[2]

[1]*Department of Semiconductor Physics, Kangwon National University*
[2]*Division of Display and Semiconductor Physics, Korea University, Sejong 30019, Korea*

Density Matrix Renormalization Group (DMRG) is a powerful tool for obtaining ground state properties of one-dimensional spin systems. Therein time evolution and dynamical properties can be studied via time-evolving block decimation (TEBD) or time-dependent variational principle (TDVP). These methods enable the calculations of real-time-dependent spin-spin correlation function, analogous to Green's functions in electron systems, and their Fourier transform $A(k, \omega)$. In gapless states, however, the long-time evolution is often prevented due to the increase in entanglement entropy as a function of time. It has been suggested that evolving time in complex number space suppresses proliferation of high-energy states and the resulting enhancement of entanglement entropy, thus enables longer-time evolution. In this study we compute the ground state properties, including magnetization, energy, and critical exponents, and spectral functions of the one-dimensional Transverse Field Ising model and XXZ model via employing the complex time evolution methods. We discuss advantages of the complex time evolution method in computational efficiency and further discuss its applicability in fermionic systems.

Poster No.2

Quantum critical transport in half-filled two-dimensional Hubbard model

Youngmin Eom and Aaram J. Kim

Department of Physics and Chemistry, DGIST, 42988 Daegu, Korea

We study quantum critical (QC) transport in half-filled two-dimensional Hubbard model using the connected determinant Monte Carlo method. Employing the stochastic optimization method for analytic continuation, we obtain the reliable optical conductivity results in the thermodynamic limit and address the metal-to-insulator crossover line associated with the antiferromagnetic QC point at the noninteracting ground state. Along the crossover line, the reflection symmetry of DC conductivity appears, and the estimated QC exponent is different from the previously reported value of the Mott transition.

Our results exclude the QC transport scenario induced by the Mott transition suggested by dynamical mean-field theory studies in infinite dimensions.

Poster No.3

Role of electron interaction and tilting angle in $Sr_3Ir_2O_7$: a model and first-principles study

Beomjoon Goh[1], Hongchul Choi[2], Ji Hoon Shim[2,3,4], and Seung-Sup Lee[1]

[1]*Department of Physics and Astronomy, Seoul National University, Seoul, 08826, Republic of Korea*
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$Sr_3Ir_2O_7$ has rich physics arising from the interplay of the spin-orbit coupling (SOC), the Coulomb interaction (U), and structural factors such as the tilting angle of the octahedron of O atoms. In this work, we study a bilayer Hubbard model, which is the minimal model of the material, with the dynamical mean-field theory (DMFT). By using the numerical renormalization group (NRG) impurity solver, we can obtain the antiferromagnetic solutions around the material's parameters without the sign problem, and resolve the electronic structure and the dynamic susceptibilities with high accuracy. Because of the interplay between the interaction and the tilting angle, a pseudogap forms, which is consistent with experiments. Interestingly, the spectral weights transfer towards the Fermi level for larger U. We also calculate the electronic Raman spectra of $Sr_3Ir_2O_7$, by plugging in the first-principles parametrization obtained from the Wannierization of the J=1/2 bands.

Poster No.4

The Quantum Zeno Monte Carlo to compute Hamiltonian eigenstate properties

Mancheon Han[1], Hyowon Park[2,3], and Sangkook Choi[1]

[1]School of Computational Sciences, Korea Institute for Advanced Study (KIAS),
[2]Materials Science Division, Argonne National Laboratory,
[3]Department of Physics, University of Illinois at Chicago

In this presentation, we introduce our quantum Zeno Monte Carlo (QZMC), a noise resilient approach that allow us to find Hamiltonian eigenstate properties within a polynomial quantum computational cost. Our algorithm implements the Quantum Zeno effect as an integral of consecutive time evolutions, which can be efficiently computed by using the Monte Carlo method. By doing so, our method computes properties of the unknown eigenstate starting from the eigenstate of easily solvable Hamiltonian. If the targeted eigenstate is energetically gapped with other states, our method can find eigenstate properties within a polynomial quantum time. Moreover, QZMC is resilient to device noise and the trotter error. By computing various eigenstate properties of one, two and many qubit systems, we demonstrate the applicability of QZMC and the noise resilience. Because the method is polynomial cost noise-resilient approach with easily preparable initial states, we expect QZMC can achieve quantum advantage within an early fault-tolerant quantum computing era.

Poster No.5

Spin Screening Clouds in Local Moment Phases

Minsoo L. Kim

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When a magnetic impurity is surrounded by conduction electrons, the impurity spin is screened via the Kondo effect. However, if the local density of states (LDOS) of electrons near the impurity exhibits a gap or divergence at the Fermi level, the screening can become imperfect, leading to the emergence of a local moment (LM) phase. Conventionally, the LM phase is understood as lacking screening. In contrast to this common belief, we show that the impurity spin is still screened by the conduction electrons. Also, the electrons screening the spin are spatially distributed, which forms a spin cloud. To show that, we calculate quantum entanglement between the impurity spin and conduction electrons, by using tensor network methods. For pseudogap and diverging LDOS, we employ the numerical renormalization group method and show that the decay of this spin cloud follows an algebraic behavior. For LDOS with a hard gap, we use the density matrix renormalization group method, and the spin cloud decays exponentially. In each case, we find that the spatial distribution of the spin cloud follows a single universal function of a rescaled distance by a characteristic length of the system.

Poster No.6

Quantum random power method for ground-state approximation

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We present a quantum-classical hybrid random power method that approximates a ground state of a Hamiltonian. The quantum part of our method computes elements of a matrix polynomial of the Hamiltonian, which is based on a quantum filtering technique that significantly improves convergence performance. This technique can be implemented using Hamiltonian simulation or block encoding, suitable for respective fault-tolerant regimes. The classical part of our method is a randomized iterative algorithm that updates the state vector on a classical computer using matrix elements computed from the quantum part. The computational cost of one iteration in our method is independent of system size. We show that with probability one, our method can converge to a good approximation of a ground state of the Hamiltonian and the quality of the approximation depends linearly on the magnitude of noise occurring from quantum computation if it is sufficiently small. Several numerical experiments demonstrate that our method provides a good approximation of ground state in the presence of systematic and/or sampling noise.

Poster No.7

Orbital-selective electron correlations and self-doped double-exchange in 1T-$CrTe_2$ with Hund metallicity

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A van der Waals ferromagnet 1T-$CrTe_2$ has recently gained significant attention for spintronic applications due to its high Curie temperature (T_C) down to atomically thin-film form, wafer-size fabrication, and intriguing transport phenomena. However, despite the importance of electron correlations intertwined with magnetism, their nature and relationship to ferromagnetism in 1T-$CrTe_2$ remain elusive. Here, we identify 1T-$CrTe_2$ as a self-doped double-exchange ferromagnet with Hund metallicity. Our density functional theory plus dynamical mean-field theory (DFT+DMFT) calculations show that all Cr-d orbitals are metallic as a consequence of self-doping, contrary to nominal configuration of two electrons in t_{2g} orbitals and band-insulating e_g states. These Cr-d orbitals exhibit strong orbital-selective correlations, where t_{2g} and e_g electrons of local moment and itinerant nature, respectively. Additionally, the t_{2g} orbitals manifest a series of Hund metallic behaviors together with Mott-like features of a half-filled t_{2g}^3 configuration, both promoting the fluctuating local moment of t_{2g} electrons. Despite the metallicity of t_{2g} states, the interplay between t_{2g} and e_g via Hund coupling J_H drives non-Fermi-liquid (NFL) behavior of e_g similar orbital-selective Mott phase (OSMP), leading to the double-exchange mechanism. These findings reveal the distinctive and complex orbital-selective correlations in 1T-$CrTe_2$, enhancing our understanding of its electronic and magnetic properties.

Poster No.8

Tensor network simulation of quantum random circuit sampling

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We develop a projected entangled pair state (PEPS) algorithm to simulate two-dimensional quantum circuits, which combines simple update gauging and graph-independent local truncations (GILT). Applied to the random circuit sampling problem proposed by Google LLC, our algorithm manifests the effective error per gate that decreases inverse-polynomially with the PEPS bond dimension. With this, we achieve lower gate errors than the state-of-the-art matrix product state (MPS) simulation. Also, by efficiently sampling one million bitstrings, we obtain the bitstring probability distribution that reproduces the Porter-Thomas (PT) distribution, considered to be intractable for approximate simulations. Overall, our result implies a possibility of reproducing random circuit sampling with classical computers within polynomial time complexity.

Poster No.9

Density Functional Theory study of CDW structure in $TiSe_2$

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1T-$TiSe_2$ is a well-studied TMDC (Transition Metal Dichalcogenide) material known for exhibiting a CDW (Charge Density Wave) at 165K. Despite extensive research, it is not clear whether this material is a semimetal or a semiconductor. Additionally, a second CDW transition at 165K has been identified. Here, we perform first-principles electronic structure calculations to investigate potential CDW patterns in 1T-$TiSe_2$ and their impact on electronic structures. When considering a 2x2x1 supercell, only a single type of CDW pattern is observed, as reported in previous theoretical studies. However, in the case of a 2x2x2 supercell, we found four different types of CDW orders, which are almost degenerate in energy. Furthermore, we utilized the band unfolding technique to compare the band structures of the four CDW phases with angle-resolved photoemission data and discussed the effects of spin-orbit coupling on the band structures. Additionally, we computed lattice-induced free energies to determine the presence of potential thermal phase transitions.

Poster No.10

Fractonic Quantum Quench in Dipole-constrained Bosons

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In this poster presentation, I will delve into the quench dynamics of the dipolar Bose-Hubbard model, a rapidly growing area in condensed matter physics that focuses on systems with preserved dipole moments. Recent studies [1] have highlighted significant progress toward the experimental realization of this model, particularly by applying sharply inclined potentials to one-dimensional bosonic systems on an optical lattice. My presentation will concentrate on the quench dynamics observed within and between different phases of this model, as detailed in [2]. The analysis will include the light-cone-like propagation of correlators, the occurrence of dynamical phase transitions, and the emergence of fidelity revivals, which are considered indicators of the many-body scar state.

[1] Ethan Lake, Hyun-Yong Lee, Jung Hoon Han, and T. Senthil1; PRB 107, 195132 (2023)
[2] Yun-Tak Oh, Jung Hoon Han, Hyun-Yong Lee; arXiv2311.13156 (2023)

Poster No.11

Metal-insulator transition of a two-orbital Hubbard-Hund system at zero temperature

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While the role of Hundness in three-orbital (t_{2g}) systems, such as Janus effect, is much understood, its role in two-orbital (e_g) systems is less elucidated. A recent dynamical mean-field theory (DMFT) study of a two-orbital model proposed that the zero-temperature metal-insulator transition can be first-order because of Hundness [1], which is different from the second-order transitions observed for symmetric three-orbital systems [2]. To fill the gap, we study the Mott transition of the two-orbital Hubbard-Kanamori model using the state-of-the-art numerical renormalization group (NRG) as a DMFT impurity solver. We demonstrate that the symmetry property of the Hund coupling is crucial; the transition is second-order as long as the SU(2) spin symmetry pertains, while it becomes first-order when there is no SU(2) symmetry.

[1] M. Chatzieleftheriou et al., Phys. Rev. Lett. **130**, 066401 (2023).
[2] K. M. Stadler, G. Kotliar, A. Weichselbaum, and J. von Delft, Ann. Phys. (N.Y.) **405**, 365 (2019).

Poster No.12

Exploring the role of *nonlocal* Coulomb interactions on the electronic structure of SrMO_3 (M = Ti - Co) perovskites: A DFT+U+V study

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We have investigated the role of *nonlocal* Coulomb interactions on the electronic structure of the SrMO_3 (M = Ti - Co) perovskites by incorporating both on-site and inter-site Coulomb interactions (DFT+U+V). The Coulomb interaction parameters are derived using constrained random phase approximation (cRPA) calculations. Our analysis reveals that the competition between localization and screening effects results in nonmonotonic behavior of screened Coulomb interaction parameters with d-orbital occupation. We emphasize the significant role and nonlocality of inter-site Coulomb interactions, V, which are comparable in magnitude to the local interaction, U. Our DFT+U+V results exemplarily show the representative band renormalization, and deviations from ideal extended Hubbard models due to increased pd-hybridization as occupation increases. We further demonstrate that the inclusion of V is essential for accurately reproducing the experimental magnetic order in transition metal oxides.

Poster No.13

Origin of the correlated gaps in twisted bilayer graphene

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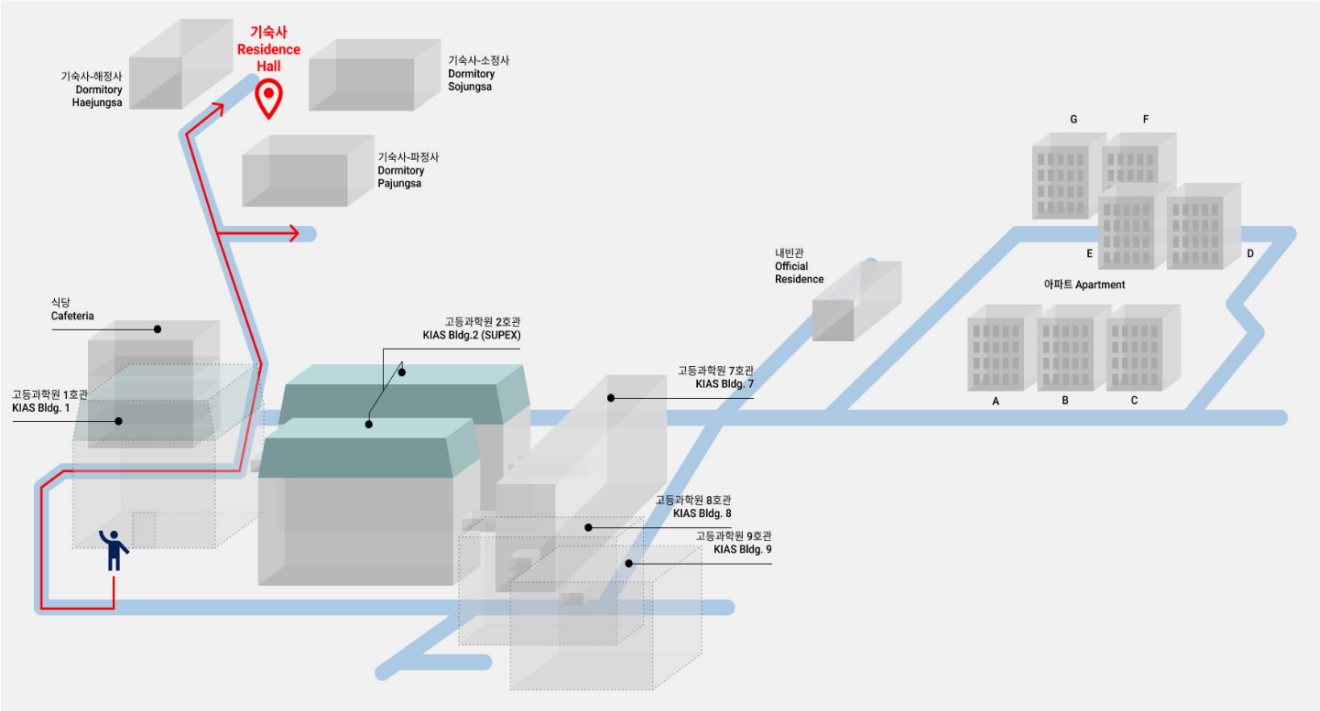
Magic-angle twisted bilayer graphene (MATBG) exhibits various strongly correlated electronic phenomena, such as correlated insulating phases and strange metal behaviors. The recently proposed topological heavy fermion (THF) model [1] and its single-valley version [2] explain the low-energy bands of MATBG by the hybridization of the interacting flat bands (f orbitals) and the topological Dirac bands [1-4]. In this work, we identify the importance of the electron-phonon coupling (EPC) [5] and the repulsion between nearest-neighbor f orbitals (parametrized by U_2) in the single-valley THF model, using the dynamical mean-field theory (DMFT) plus the Hartree mean-field approach. With our state-of-the-art numerical renormalization group (NRG) impurity solver, we obtain the spectral function, the dynamic susceptibilities, and the resistivity with unprecedented resolution and accuracy. We find that including EPC is necessary for explaining more pronounced gaps at $\nu \simeq \pm 2$ than $\nu \simeq \pm 1, \pm 3$ as observed in experiments. On the other hand, larger U_2 suppresses the gaps for all ν's. The intricate competition between the EPC and the U_2 term may imply the sample-dependent phase diagrams of MATBG.

[1] Z.-D. Song and B. A. Bernevig, Phys. Rev. Lett. 129, 047601 (2022).
[2] G.-D. Zhou et al., Phys. Rev. B 109, 045419 (2024).
[3] H. Hu et al., Phys. Rev. Lett. 131, 026502 (2023).
[4] G. Rai et al., arXiv:2309.08529.
[5] Y. Wang et al., arXiv:2402.00869.

Bldg.1 to Residence Hall



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3. You will see KIAS(KAIST campus) across the street.