PROGRAM AND ABSTRACTS

Computational Quantum Many-Body Theory

July 6 – 8, 2026

Rm. 1503, KIAS, Seoul

Plenary Speakers

Naoki Kawashima (U of Tokyo)

Sandeep Sharma (Caltech)

Sergey Y. Savrasov (UC Davis)

Invited Speakers

Aaram J. Kim (DGIST)

Donghoon Kim (RIKEN)

Erik van Loon (Lund University)

Hyun-Yong Lee (Korea University)

Joonho Lee (Harvard University)

Masato Kobayashi (Hokkaido University)

Min-Cheol Kim (Sookmyung Women's University)

Moon Jip Park (Hanyang University)

Myung Joon Han (KAIST)

Seunghoon Lee (Seoul National University)

Tsuyoshi Okubo (University of Tokyo)

Zhengcheng Gu (CUHK)

Session Chairs

Dong-Hee Kim (GIST)

Dong Yeon Kim (Jeonbuk National University)

Heung-Sik Kim (Kentech)

Hongkee Yoon (Kangwon National University)

Minho Kim (Kyung Hee University)

Organizing Committee

Hyun-Yong Lee (Korea University)

Myung-Joon Han (KAIST)

Sangkook Choi (KIAS)

Seunghoon Lee (Seoul National University)

Computational Quantum Many-body Theory

	July 6 (Mon)	July 7 (Tue)	July 8 (Wed)
9:00-9:30	Registration		
9:30-10:30	**Chair: Dong Yeon Kim**	**Chair: Heung-Sik Kim**	**Chair: Hongkee Yoon**
	Sandeep Sharma	Sergey Y. Savrasov	Naoki Kawashima
10:30-11:10	Joonho Lee	Myung Joon Han	Moon Jip Park
11:10-11:50	Zhengcheng Gu	Seunghoon Lee	Tsuyoshi Okubo
11:50-13:30	**Lunch**		
13:30-14:10	**Chair: Dong-Hee Kim**	**Excursion and Dinner**	**Chair: Minho Kim**
	Erik van Loon		Hyun-Yong Lee
14:10-14:50	Aaram J. Kim		Min-Cheol Kim
14:50-15:30	Masato Kobayashi		Donghoon Kim
15:30-16:00	Coffee Break		
16:00-18:00	**Poster Session**		
18:00-20:00	**Banquet**		

ABSTRACTS OF TALKS

Title: Optimization of Tensor Network for Machine Learning

Abstract: We proposed adaptive tensor tree [1], a method for constructing Born machine [2] on a tensor tree that infers the distribution function from observed samples. The distribution functions are expressed as the amplitude of a tensor-tree wave function. The tensors are optimized to minimize the negative log-likelihood, i.e., the Kullback-Leibler divergence of the sample distributions from the tensor-tree distribution. In contrast to many neural-network-based generative models, in this scheme, the branching structure is also optimized. It is done by detecting branches of heavy information traffic --- high bond mutual information (BMI) --- and reconnecting branches so as to reduce the burden. The scheme is applied to the data taken from the stock prices of the companies included in the S&P500 index, which then produced a network structure reflecting the industry categories of the componies. A drawback of the original ATT scheme, though, was that we cannot interprete the sub-network as representing causal relation (i.e., conditional probability) because the sub-network is not necessarily expressed in non-negative real numbers. To correct this drawback, we [3] attempted to extend the ATT to a single non-negative network, which is advantageous for detecting relational structures between hidden random variables. We examined the methods in several examples including the mitocondrial DNA to reconstruct the phylogenetic tree of animals.

[1] K. Harada, T. Okubo and N. Kawashima: Machine Learning: Science and Technology, 6 (2025) 025002.
[2] S. Cheng, J. Chen, and L. Wang: Entropy 20, 583 (2018).
[3] K. Akamatsu, K. Harada, T. Okubo and N. Kawashima: Machine Learning: Science and Technology 7 (2026) 015014..

Wavefunction methods for electrochemistry

Sandeep Sharma

Division of Chemistry and Chemical Engineering, California Institute of Technology

I am developing new high-accuracy electronic-structure methods aimed at predictive simulations of electrochemical systems. A central focus is auxiliary-field quantum Monte Carlo (AFQMC) algorithms that combine systematically improvable accuracy with linear-scaling cost, numerical stability for metallic systems, and robustness in strongly correlated regimes. These capabilities are designed to address key challenges in electrochemistry, where transition-metal centers, electrode surfaces, solvated interfaces, and near-degenerate electronic states often limit the reliability of conventional methods. In parallel, I am developing analytic nuclear gradients for local CCSD(T), enabling accurate geometry optimization, reaction-path characterization, and force-based simulations at reduced cost. Together, these advances aim to make benchmark-quality quantum chemistry feasible for realistic electrochemical reactions, catalytic intermediates, and electrode–electrolyte interfaces.

Towards first-principle predictions of unconventional superconductivity

Sergey Savrasov

University of California Davis

I will overview our recent works on diagonalizing BCS gap equation for a series of unconventional superconductors, where the matrix elements of scattering between the Cooper pairs are calculated from first-principle evaluation of the RPA type expression based on density functional derived band structures and wave functions. This approach has an advantage of not involving tight-binding approximations of any sort that was widely employed in the past to calculate spin fluctuations in high-T_c materials. Superconducting energy gaps, Eliashberg spectral functions, and material specific coupling constants will be evaluated for a series of cuprates, nickelates and recently discovered Kagome based vanadates. Perspective will be given how far we are from predicting material dependent Tc's in unconventional superconductors similar to past developments to explore electron-phonon superconductivity.

Diagrammatic interpretation of bad-metallic transport in 2D Hubbard model

Aaram J. Kim

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

We study the incoherent charge transport in the prototypical two-dimensional Hubbard model from the viewpoint of diagrammatic decomposition. Using the numerically exact diagrammatic Monte Carlo method, we calculate the dynamical current–current correlation function in the thermodynamic limit and perform analytic continuation to obtain the optical conductivity using the method of stochastic optimization with consistent constraints. Our analysis reveals an unconventional $T^{-1/2}$ dependence of the diffusion constant over a wide range of temperatures and interaction strengths, where the DC resistivity exhibits anomalous T or $T^{-1/2}$ scaling. This behavior is consistent with recent results from ultracold atom experiments. At low temperatures, we observe a pseudogap metal with mixed characteristics of both metallic and insulating behavior and demonstrate the pronounced role of vertex diagrams in this regime.

Entanglement area law in interacting bosons: from the Bose-Hubbard model, ϕ^4 theory, and beyond

Donghoon Kim

RIKEN Center for Quantum Computing

The entanglement area law is a fundamental principle that characterizes the structure of quantum correlations in many-body systems and plays a central role in the success of tensor-network algorithms. Rigorous proofs of the area law for ground states have traditionally relied on two key assumptions: bounded local energy and short-range interactions. Extending such results to bosonic systems, where the local Hilbert space is unbounded, and interactions may be long-range, remains a major challenge. In this work, we establish the entanglement area law for a broad class of one-dimensional interacting bosonic systems, including the Bose-Hubbard and ϕ^4 models, as well as systems with long-range interactions [1]. Our approach overcomes the limitations of the standard assumptions by proving subexponential decay of the boson-number distribution induced by interactions. As a consequence, we show that the ground states of these systems can be approximated by Matrix Product States (MPS) with quasi-polynomial bond dimension. These results provide a rigorous foundation for tensor-network simulations of interacting bosonic systems with unbounded local degrees of freedom and long-range interactions.

[1] **D. Kim** and T. Kuwahara, "Entanglement area law in interacting bosons: from Bose-Hubbard, ϕ^4, and beyond," arXiv:2411.02157.

Modelling Quantum Materials: interactions beyond Hubbard's U

Erik van Loon

NanoLund and Division of Mathematical Physics, Physics Department, Lund University, Lund, Sweden

LINXS Institute of advanced Neutron and X-ray Science (LINXS), Lund, Sweden

Wallenberg Initiative Materials Science for Sustainability

Model Hamiltonians such as the Hubbard model play a central role in quantum many-body theory for materials. Despite its simple form and small number of parameters, this model can capture a wide variety of correlation phenomena. By now, great progress has been made in computationally solving the Hubbard model and its multiorbital generalizations. However, in reality the screened Coulomb interaction in quantum materials is quite different from the Hubbard model, it is nonlocal in both space and time. In this talk, I will discuss how to calculate these nonlocal interactions, how to handle them in computational workflows and what impact they have on phase transitions and collective excitations. Finally, I will present the Nb_3X_8 (X=F,Cl,Br,I) family of materials, where the correlated orbitals are molecular in nature. This family provides a promising platform for many-body engineering.

[1] Aretz et al., Phys. Rev. X **15**, 041042 (2025)

Universal Information-Theoretic Structure of the Quasi-Stationary Domany–Kinzel Automaton

Hyun-Yong Lee

Department of Applied Physics, Korea University, Sejong, Korea;
Institute for Solid State Physics, The University of Tokyo, Japan

Directed percolation is the canonical universality class for nonequilibrium transitions into absorbing states, and the Domany–Kinzel cellular automaton is its minimal realization. On any finite chain the dynamics is ultimately trapped in the empty absorbing state, so the physically meaningful object is the quasi-stationary distribution (QSD) — the distribution of configurations conditioned on survival. We obtain the full QSD as a matrix-product state by power iteration of the projected transfer matrix; this yields the probability of every configuration explicitly, together with exact rejection-free sampling, and thereby grants access to information-theoretic diagnostics that moment- and sampling-based methods cannot reach. We find that the inactive-phase QSD behaves as a single "flock": although the surviving activity is geometrically fragmented into several clusters separated by holes, the bipartite mutual information across the chain collapses to a single bit — the left–right position of one bound object — even though the directly counted number of clusters is much larger. Approaching the critical point, the flock loosens and spreads while remaining a single positional degree of freedom. The approach opens an information-theoretic characterization of absorbing-state quasi-stationary distributions.

Ab Initio Materials Modeling When Material Specificity Matters

Name

Joonho Lee

Affiliation

Harvard University

In this talk, I will discuss our group's recent efforts in ab initio simulations of polarons and correlated materials. With a few technical developments on the algorithm side, I argue that we are ready to tackle some of the more sophisticated ab initio modeling problems. I will also highlight some successful instances in which material specificity has qualitatively changed our microscopic understanding.

Large-scale quantum chemical methods for statically correlated systems

Masato Kobayashi

Faculty of Science and WPI-ICReDD, Hokkaido University, Sapporo, Japan

We have developed divide-and-conquer (DC) linear-scaling quantum chemical methods, particularly for mean-field (i.e., HF/DFT) and dynamical electron correlation theories [1]. However, describing strong (or static) electron correlation in large systems based on the fragmentation approach remains challenging. This presentation introduces our recent attempts to treat statically correlated systems via the DC method.

1. DC Hartree–Fock–Bogoliubov (HFB) method

The HFB method, originally developed as a mean-field theory for Bogoliubov quasiparticles and applied to electronic structure in Ref. [2], is related to the geminal-based wavefunction, which can describe the static electron correlation. We have proposed the DC-HFB method [3] as an efficient static correlation theory for large systems and derived its energy gradient for the enabling geometry optimization [4].

2. DC projected unrestricted Hartree–Fock (PUHF) method

Although unrestricted HF (UHF) energy can also be used to approximate the static electron correlation, the UHF wavefunctions suffer from spin contamination. Applying the projection operator to these wavefunctions can extract the desired spin state [5]. We are currently developing a DC-based projected UHF method [6].

3. DC electron correlation calculation on quantum computer

The variational quantum eigensolver (VQE) is a widely used method for quantum chemical computations on quantum computers. Yoshikawa *et al.* [7] proposed the DC-VQE method to reduce the number of qubits and quantum gates required for large systems. In collaboration with Prof. Yoshikawa, we examined the practical performance of the DC-VQE method on the non-error-tolerant quantum devices.

[1] H. Nakai, *MK et al.*, *J. Phys. Chem. A* **127**, 589 (2023).
[2] V.N. Staroverov and G.E. Scuseria, *J. Chem. Phys.* **117**, 11107 (2002).
[3] *MK* and T. Taketsugu, *Chem. Lett.* **45**, 1268 (2016).
[4] *MK*, R. Kodama, T. Akama, and T. Taketsugu, *Chemistry* **7**, 46 (2025).
[5] C.A. Jiménez-Hoyos *et al.*, *J. Chem. Phys.* **136**, 164109 (2012).
[6] T. Yoshikawa, S. Kasaya, M. Nishida, T. Taketsugu, and *MK*, *in revision*.
[7] T. Yoshikawa, T. Takanashi, and H. Nakai, *J. Chem. Theory Comput.* **18**, 5360 (2022).

Density Functional Theory for Catalytic and Electrocatalytic Reactions

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Nowadays, the global environmental crisis including fossil fuel depletion and global warming has become a severe problem. To overcome these issues, renewable and green energy sources are of great interest, and hydrogen energy is one of the most promising methods to achieve green energy. The hydrogen industry consists of various important processes related to hydrogen, including fuel cells, hydrogen production, and conversion. These processes involve chemical reactions from one chemical substance to another chemical substance, and these reactions can be accelerated with electrocatalysts. Therefore, designing novel catalysts and electrocatalysts is essential to realize a true renewable and green energy process.

In silico materials design is a powerful and practical tool for designing novel materials using quantum chemical simulations such as the density functional theory (DFT), which can significantly reduce the cost than trial-and-error bases experimental approaches and enables rational design of energy materials. In this presentation, I introduce how to utilize quantum chemical simulations techniques to provide novel design strategies for hydrogen production catalysts and ammonia-mediated hydrogen conversion catalysts.

Unconventional superconductivity in non-collinear magnets

Moon Jip Park

(Hanyang university)

Altermagnet is an exotic class of magnetic materials wherein the Fermi surface exhibits a momentum-dependent spin-splitting while maintaining a net zero magnetization. Previous studies have shown that this distinctive spin-splitting can induce chiral p-wave superconductors or Fulde-Ferrell (FF) superconducting states carrying finite momentum. However, the underlying mechanisms of such unconventional superconductivities remain elusive. Here, we propose that the formation of the Bogoliubov Fermi surface (BFS) through the exchange field can play a significant role in such phenomena. Through a systematic self-consistent mean-field analysis on the extended attractive Hubbard model combined with the d-wave spin-splitting induced by the exchange field, as observed in RuO2, we demonstrate that the formation of the BFS suppresses conventional spin-singlet superconducting states with s-wave characteristics. In contrast, the chiral p-wave state maintains a fully gapped spectrum without the Fermi surface, thereby becoming the ground state in the strong field regime. In the intermediate regime, we find that the FF state becomes the predominant state through the optimization of available channels for Cooper pairing. Moreover, we illustrate how the prevalence of the chiral p-wave and FF states over the s-wave state changes under the variation of the field strength or chemical potential. Our findings provide valuable insights into potential pathways for realizing sought-after topological p-wave superconductivity and finite momentum pairing facilitated by altermagnetism.

Discovering Novel Magnetic Phases via Magnetic Force Theory and AI-Driven Materials Design

Myung Joon Han

Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Korea

In this talk, I present a unified framework for discovering novel magnetic materials by integrating magnetic force response theory (MFT), high-throughput first-principles calculations, and emerging AI-driven materials design strategies. We first develop an ab-initio high-throughput approach to identify frustrated magnetic systems on Kagome and triangular lattices. By combining density functional theory with MFT-based exchange interaction analysis and effective spin Hamiltonians, we systematically screen insulating 3d transition-metal compounds. This approach not only reproduces known frustrated magnets but also predicts previously unexplored candidates, revealing magnetic ground states governed by competing exchange interactions and lattice geometry. Building on the noncollinear extension of MFT, we further establish a multi-scale workflow to explore emergent topological spin textures. By integrating first-principles-derived magnetic interactions with atomistic spin simulations, we perform a comprehensive search across monolayer transition-metal dichalcogenides with diverse crystal structures and compositions. This approach uncovers a wide range of noncollinear and topologically protected spin configurations, including skyrmions and bimerons, and elucidates their microscopic stabilization mechanisms. Finally, we extend our discovery paradigm beyond existing materials databases by incorporating generative AI techniques. Using a diffusion-based crystal generation model combined with targeted screening and first-principles validation, we identify new candidate altermagnets—an emerging class of magnetic materials characterized by zero net magnetization and momentum-dependent spin splitting. Starting from tens of thousands of generated structures, we apply symmetry compatibility tests, AI classification, and DFT+U validation to isolate robust candidates. This workflow yields several previously unknown altermagnets, including systems exhibiting sizable spin splitting, demonstrating the effectiveness of integrating generative models with physics-based screening. Together, these results establish a scalable and predictive platform for magnetic materials discovery, bridging fundamental theory and data-driven design, and opening new pathways toward realizing unconventional magnetic phases.

Excited-State Dynamics Simulations in Extended Systems Using Embedded Many-Body Excited-State Method

Nakhyun Kim,† Cheol-Ho Choi,‡ YounJoon Jung,† and Seunghoon Lee†

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‡*Department of Chemistry, Kyungpook National University, Daegu 41566, South Korea*

Controlling excited-state dynamics associated with excitations localized at surface sites, molecular units, or defects in extended materials has attracted growing interest. This capability is essential for enhancing photocatalytic efficiency, optimizing charge-transfer and recombination processes in optoelectronic materials, and improving the optical performance of color centers in solid-state quantum-information platforms. Achieving such control requires a microscopic understanding of how spatially localized excitations evolve while coupled to lattice vibrations and the surrounding material environment.

Mixed quantum–classical surface-hopping approaches are used to describe the nonadiabatic dynamics of spatially localized excitations in extended materials. Recent approaches have combined surface hopping with many-body excited states obtained from linear-response time-dependent density-functional theory (LR-TDDFT). Although this approach can better capture processes that require an explicit many-body excited-state description, it relies on computationally demanding calculations of dense manifolds of LR-TDDFT states within supercells and inherits the well-known limitations of LR-TDDFT for excited-state dynamics.

In this work, we propose a new theoretical model that addresses these two challenges by combining a local excited-state representation with mixed-reference spin-flip (MRSF)-TDDFT. This model is specifically designed for such cases where competing localized excited-state pathways evolve on comparable time scales, making strong electronic correlation essential. Instead of constructing dense manifolds of many-body excited states for the full supercell, we restrict the excited-state description to the local region in which the competing pathways occur. This reduction is motivated by the observation that nonadiabatic couplings are strongest between states with substantial spatial overlap in their excitation amplitudes. At the same time, MRSF-TDDFT mitigates key limitations of conventional LR-TDDFT for excited-state dynamics in situations involving bond breaking and formation, ground- and excited-state conical intersections, open-shell diradical character, and double-excitation character.

Tensor-network approaches to finite-temperature phenomena in frustrated quantum spin systems

Tsuyoshi Okubo

Department of Physics, Niigata University

Department of Physics, University of Tokyo

Tensor-network methods have become powerful tools for investigating strongly correlated quantum many-body systems, providing access not only to ground-state properties but also to finite-temperature and dynamical phenomena. In this talk, I will discuss tensor-network approaches to finite-temperature phenomena in frustrated quantum spin systems, with a focus on direct tensor-network representations of thermal density matrices. In particular, I will consider single-layer representations, such as matrix product operators and tensor product operators, and their optimization at finite temperatures.

Finite-temperature phase transitions in extended Kitaev models on the honeycomb lattice provide a representative example of this approach. Tensor product operator representations of thermal density matrices are used to investigate temperature-driven ordering phenomena associated with the breaking of lattice rotational symmetry. This demonstrates that finite-temperature tensor-network methods can directly address phase transitions in two-dimensional frustrated quantum spin systems.

Another application concerns thermal Hall transport in extended Kitaev models under a magnetic field. Using finite-temperature tensor-network calculations with open boundary conditions, the thermal Hall conductivity is computed and its temperature and field-direction dependence are analyzed. The calculated thermal Hall conductivity divided by temperature exhibits a pronounced hump upon cooling, consistent with experimental observations in the Kitaev candidate material α-$RuCl_3$.

As a further example, the thermal Hall response of the kagome-lattice Heisenberg model with Dzyaloshinskii–Moriya interaction under a magnetic field is briefly discussed. Magnetization plateaus, including the 1/9 and 1/3 plateaus, are stabilized even at finite temperatures, and the thermal Hall conductivity exhibits distinct temperature dependences at these plateaus. These examples demonstrate the usefulness of finite-temperature tensor-network methods as computational tools for exploring phase transitions, thermal transport, and exotic quasiparticle signatures in frustrated quantum spin systems.

Pseudogap phase as fluctuating pair density wave

Zhengcheng Gu

The Chinese University of Hong Kong

The physical nature of pseudogap phase is one of the most important and intriguing problems towards understanding the key mechanism of high temperature superconductivity in cuprates. Theoretically, the square-lattice t-J model is widely believed to be the simplest toy model that captures the essential physics of cuprate superconductors. We employ the fermionic tensor network state approach to investigate uniform states in the underdoped ($\delta \lesssim 0.1$) region. In addition to the previously known uniform d-wave state, we discover a strongly fluctuating pair density wave (PDW) state with wave vector $Q = (\pi, \pi)$. This fluctuating PDW state weakly breaks the C_4 rotational symmetry of the square lattice and has a comparable or lower energy to the d-wave state (depending on doping and the t/J ratio), making it a promising candidate state for describing the pseudogap phase. If time permits, I will also discuss our recent results on the origin of experimentally observed $4a_0$ pattern from interference between the various PDW states and uniform d-wave state.

ABSTRACTS OF POSTERS

Poster No. 1

AI-guided high-throughput discovery of new altermagnet candidates

Jiwon Choi, Yuhyun Cha, Myung Joon Han*

Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Korea

In this study, we present a high-throughput discovery workflow integrating diffusion-based crystal generation, AI-based altermagnet pre-screening, and first-principles validation to identify new altermagnet candidates. Starting from 51,200 generated structures, we downselect candidates using an AI classifier and symmetry-compatibility assessment. We then validate the altermagnetic ground state by density functional theory (DFT)+U total energy comparisons among competing magnetic configurations. This workflow yields eight new altermagnets, and their spin splittings are benchmarked against 90 known altermagnets. Notably, $NiCO3$ ($P2_1$) and $OHFe_2F_5$ (Amm2) are identified as particularly strong candidates, encompassing both stable and potentially synthesizable metastable phases. Our results demonstrate that integrating generative models with targeted screening and DFT validation enables efficient discovery of new altermagnet candidates.

Poster No.2

Comparative Analysis of cRPA Methods for Calculating Hubbard *U* Parameters

Indukuru Ramesh Reddy[1], M. Kaltak[2], and Bongjae Kim[1,*]

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We present a systematic study of the calculation of Coulomb interaction parameters, specifically focusing on the Hubbard *U*, using the constrained random-phase approximation (cRPA). A key challenge arises from the different ways of defining the correlated subspace and performing projections, especially in systems with entangled bands, where different projection schemes from hybridized bands to the correlated subspace can yield varying sizes of interaction parameters. We systematically evaluate different approaches to construct the Wannier basis for extracting the correlated subspace from Kohn-Sham orbitals, addressing the challenges associated with defining the correlated basis. We then compare *U* values from various cRPA approaches, highlighting their distinct advantages and challenges related to screening accuracy and consistency. To illustrate these effects, we study two representative family of *d*-orbital oxides: LiMO$_2$ (M = V - Ni) as examples of systems with isolated *d*-bands, and SrMO3 (M = Mn, Fe, and Co) as cases of entangled *d*-bands. Through this systematic comparison, we provide a detailed analysis of different cRPA methodologies for computing the Hubbard parameters [1,2].

[1] I. R. Reddy, M. Kaltak, and B. Kim, Phys. Rev. B 111, 195144 (2025).

[2] M. Kaltak, A. Hampel, M. Schlipf, I. R. Reddy, B. Kim, and G. Kresse, Phys. Rev. B 112, 245102 (2025).

Poster No.3

Mott transition in multi-orbital Hubbard models: transition orders and unstable Fermi-liquid solutions

Sanghyun Park[1] and Seung-Sup B. Lee[1,2,3]

[1]*Dept. of Physics and Astronomy, Seoul National University, Seoul 08826, Korea*

[2]*Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea*

[3]*Institute for Data Innovation in Science, Seoul National University, Seoul 08826, Korea*

In this work, we investigate multi-orbital Hubbard models with Hund's coupling within dynamical mean-field theory, using the numerical renormalization group as a real-frequency impurity solver. We show that the local ground-state degeneracy (D_g) plays a central role in determining the transition order characterized by the behavior of the quasiparticle weight Z. The zero-temperature transition is first-order when $D_g < M + 1$, while it becomes continuous when $D_g \geq M + 1$, where M is the number of the orbital. We further demonstrate that the unstable solutions inside the coexistence region are Fermi liquids, but with stronger mass renormalization than the stable metallic solution. Finally, we revisit the finite-temperature unstable branch of the one-band Hubbard model and identify quantum-critical scaling associated with the underlying zero-temperature Mott criticality.

Poster No.4

Anisotropy-induced non-Fermi-liquid fixed points in the two-channel spin-orbital Kondo models

Hyunsung Jeong[1], Sanghyun Park[1] and Seung-Sup B. Lee[1,2,3]

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The Kondo model serves as a paradigmatic framework for describing strongly correlated quantum systems and has been extensively studied in both bulk materials and mesoscopic devices such as quantum dots [1, 2]. Generalized Kondo models, including multi-channel [3] and multi-impurity [4] variants, are known to host non-Fermi-liquid (NFL) behavior beyond the Landau Fermi-liquid paradigm. In this work, we investigate two-channel spin-orbital Kondo models in which the impurity carries an additional orbital degree of freedom. Using the numerical renormalization group (NRG), we solve both the isotropic and anisotropic models and map out the global phase diagram. We identify two anisotropy-induced NFL fixed points: an orbital ferromagnetic NFL and an $SU(2)\times \mathbb{Z}_2$ spin-orbital NFL. We further characterize the fixed-point structure using the NRG finite-size spectra and the low-energy power-law behavior of various dynamical susceptibilities. These exponents are interpreted via boundary conformal field theory, using the spectator fusion technique recently introduced for the three-channel spin-orbital Kondo model [5]. Our results show that orbital anisotropy enriches the landscape of spin-orbital Kondo physics and can stabilize distinct NFL behavior beyond the isotropic limit.

[1] J. Kondo, *Prog. Theor. Phys.* **32**, 37 (1964).
[2] D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu et al., *Nature* **391,** 156 (1998).
[3] Ph. Nozières and A. Blandin, *J. Phys*. (France) **41**, 193 (1980).
[4] B. A. Jones and C. M. Varma, *Phys. Rev. Lett*. **58**, 843 (1987).
[5] E. Walter, K. M. Stadler, S.-S. B. Lee et al., *Phys. Rev. X.* **10**, 031052 (2020).

Poster No.5

Quantifying Uncertainty of Admissible Solutions in Analytic Continuation

KyungKyu OH[1], AaRam J. KIM[2*], HongKee YOON[1*]

[1]*Department of Physics, Kangwon National University, Chuncheon*

2Department of Physics and Chemistry, DGIST, Daegu

Analytic continuation—reconstructing real-frequency spectral functions from imaginary-time Green's functions—is an inherently ill-posed inverse problem highly sensitive to statistical noise. Various methods have been developed, including Maximum Entropy Method (MEM) [1], Padé approximants [2], stochastic analytic continuation (SAC) [3], Nevanlinna method [4], projection, pole estimation, and semidefinite relaxation (PES) [5–8], and machine-learning approaches [9,10]. While these methods can produce candidate spectral functions, they generally lack a principled way to quantify solution uncertainty. In particular, estimating the range of admissible solutions that are consistent with the input data has remained difficult, making it hard to judge whether a result is physically reasonable or to compare candidates across different methods. To address this, we propose a framework for quantitative uncertainty assessment in analytic continuation. Under the prior assumption that physical spectral functions are smooth and continuous, we adopt a B-spline parameterization [11] and systematically perturb key spectral features such as peak heights and widths to construct explicit error bars and error maps. These error measures delineate the "reasonable" region of solution space and enable systematic comparison of uncertainty across different spectra, noise levels, and constraints.

[1] Bergeron, D. & Tremblay, A.-M. S. Phys. Rev. E 94, 023303 (2016).
[2] Schött, J. et al. Phys. Rev. B 93, 075104 (2016).
[3] A. W. Sandvik, Phys. Rev. B 57, 10287 (1998).
[4] Fei, J., Yeh, C.-N. & Gull, E. Phys. Rev. Lett. 126, 056402 (2021).
[5] Huang, Z. et al. Phys. Rev. B 107, 075151 (2023).
[6] Fei, J.et al. Phys. Rev. B 104, 165111 (2021).
[7] Zhang, L. & Gull, E. Phys. Rev. B 110, 035154 (2024).
[8] Yoshimi, K. et al. Comput. Phys. Commun. 244, 319–323 (2019).
[9] Yoon, H. et al. Phys. Rev. B 98, 245101 (2018).
[10] Fournier, R et al. Phys. Rev. Lett. 124, 056401 (2020).
[11] Chaudhuri, A. arXiv preprint arXiv:2108.06617 (2021).

Poster No.6

Disentangled Quantic Tensor Cross Interpolation

Jeong Hyeok Cha[1], and Seung-Sup B. Lee[1]

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Quantics Tensor Cross Interpolation (QTCI) provides an efficient tensor-network representation of high-resolution functions by encoding physical coordinates into binary degrees of freedom and constructing a tensor train directly from sampled function values. Although QTCI is effective for many structured functions, its efficiency can deteriorate when the target function develops strong correlations across the binary variables, leading to large tensor-train bond dimensions. To address this limitation, we introduce a disentangling scheme based on invertible bit-string transformations generated from a GL(2,2)-based binary gate set. By reorganizing the binary coordinates before interpolation, this procedure seeks a representation in which the same sampled function admits a more disentangled tensor-train structure. We show that this disentangling approach improves the compression of otherwise high-rank functions at comparable accuracy, reducing the required bond dimensions and extending the practical applicability of QTCI to more challenging high-resolution functions.

Poster No.7

Telum.jl: A Julia-based non-Abelian tensor library with exact Clebsch–Gordan data

Kiyeon Kim[1,2] and Seung-Sup Lee[1,2,3]

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Telum.jl is a non-Abelian tensor network library written entirely in Julia. Its internal Clebsch–Gordan engine, LurCGT.jl, extends the approaches of QSpace and TensorKit.jl to compute symmetry-related quantities for SU(N), Sp(2N), SO(N), and G2 exactly using integer arithmetic and in a deterministic manner. Telum.jl is designed to handle tensors with arbitrary combination of these symmetries, with ready-to-use support for spinful fermionic spaces involving U(1), SU(2), and SU(N) charge, spin, and channel symmetries.

Telum.jl is designed for users to implement high-performance tensor network algorithms with simple and readable syntax. It provides an ITensor-style interface, together with utility methods for explicitly controlling contracted legs. On the performance side, Telum.jl implements an efficient SVD algorithm that avoids explicit leg fusion, as well as lazy evaluation for simple operations such as conjugation. In benchmark calculations performed so far, Telum.jl achieves CPU runtimes comparable to QSpace while reducing memory usage. Further optimizations, including lazy evaluation for tensor contractions and GPU support, are planned for future releases.

Poster No. 8

Solving finite-difference parquet equations using quantics tensor trains

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We present a scalable numerical scheme to solve the parquet equations, a set of self-consistent relations between two-particle vertex functions. We employ a recently developed finite-difference method that bypasses vertex divergences that can arise when non-perturbative input is used, e.g., in dynamical vertex approximation (DΓA) applications. By compressing correlation functions into quantics tensor trains (QTTs), data on large, dense Matsubara frequency grids can be efficiently stored and manipulated. Our solver supports three different modes of treating momenta: full momentum resolution, s-wave approximation, and multi-mode form-factor expansions. We benchmark our parquet approximation and DΓA results for the single-impurity Anderson and 2D Hubbard models against established data, such as those from numerical and functional renormalization group calculations.

Poster No.9

Diagrammatic interpretation of transport in 2d doped Hubbard model

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We study the strange metallic charge transport in the 2d doped Hubbard model using diagrammatic Monte Carlo method. Using the double-series expansion of the current-current correlation function and performing analytic continuation in a controlled manner, we obtain the optical conductivity directly in the thermodynamic limit at the optimal doping.

It turns out that, upon doping, the antiferromagnetic insulator at half filling evolves into a bad metallic state with the coexistence of the central Drude peak and the high-energy satellite.

Furthermore, by measuring the current structure factor, we reveal the hidden spatial fluctuations underlying the optical response.

Poster No. 10

Effect of Potential Drop Direction on Mott Gap Closing in Hubbard Model: Cluster DMFT Study

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Mott gap closing by on-site potential difference is studied by 2x2 plaquette cluster DMFT in the half-filled Hubbard lattice. The potential drop of ~0.6 |t| along one bond direction, i.e. [10], is shown to stabilize the metallic phase over the Mott insulators whose Coulomb repulsion is equal to U = 5.8 |t|. When the potential varies along the diagonal direction ([11]), the same transition occurs at ~0.6|t|/sqrt(2) for the drop per bond. This could indicate the electric field strength rather than on-site potential difference per bond as the key parameter to cause transition from the Mott insulator to correlated metals. Nevertheless, the antiferromagnetically correlated metallic state exhibits lower scattering rate for [11] than [10] potential variation. Relevant features in the spectral function and further effect of the potential drop direction are analyzed.

Poster No. 11

Direction-selective intertwined charge, orbital, and lattice orders under uniaxial strain in hole-doped manganite: $La_{0.75}Ca_{0.25}MnO_3$

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Abstract

The complex interplay of charge, spin, orbital, and lattice degrees of freedom governs emergent phases in quantum materials, making strain a powerful control parameter. Recent advances in freestanding layer techniques have enabled extreme strains of nearly 8%, opening access to novel and often unexpected electronic and magnetic phases.

Here, using a density functional theory approach, we investigate the effect of direction-selective uniaxial strain on the prototypical Jahn-Teller system $La_{1-x}Ca_xMnO_3$ ($x = 0.25$). We find that different strain directions stabilize qualitatively distinct structural, charge, and orbital responses, rather than merely different strengths of the same phase. In particular, extreme uniaxial strain selectively induces cooperative Jahn-Teller, breathing-like, and site-selective modulations, thereby enabling previously inaccessible intertwined orders in manganites. These results establish direction-selective uniaxial strain as a powerful and selective route for engineering emergent phases in quantum materials.

Poster No. 12

QAssemble: A Pure Python Package for Quantum Many-Body Theory

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QAssemble is a pure-Python package for the quantum many-body problem, implementing tight-binding, Hartree–Fock, and GW approximations within a unified object-oriented architecture. Each physical concept—crystal structure, Hamiltonian, Green's function, self-energy, polarizability, and screened Coulomb interaction—is represented as a distinct class, built on NumPy, SciPy, and libdlr. Performance-critical kernels, including the polarizability bubble, Dyson-equation inversion, and lattice Fourier transforms, are systematically vectorized and combined with the discrete Lehmann representation to achieve practical efficiency within a pure-Python environment. Validated on the electronic structure of graphene with local and non-local interactions, QAssemble delivers up to a 60× speedup over traditional loop-based Matsubara implementations on a five-orbital extended Hund–Hubbard model, while supporting both batch execution for production calculations and interactive workflows for method development.

Poster No. 13

Disorder-driven complexity transitions in a quantum advantage architecture

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While decoherence is known to erode the classical hardness in quantum random sampling, the impact of coherent spatial disorder remains an open question. We study a square-lattice instantaneous quantum polynomial-time (IQP) architecture subject to two-qubit gate-angle disorder and single-qubit dephasing using exact tensor-network simulations up to 576 qubits. For finite systems without dephasing, increasing disorder drives two consecutive crossovers restoring classical simulability: anticoncentration first breaks down, and then the simulation costs drop from exponential to polynomial due to suppression of entanglement. The finite-size scaling analyses reveal that the crossovers become phase transitions in the large-system limit. Dephasing further reduces the complexity. We characterize the computationally hard regime with various scaling behaviors, which can provide quantitative error-budget bounds for realistic near-term devices

Poster No. 14

Title: Estimating dynamical correlation functions using quantum simulations with adaptive measurement techniques

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Dynamical correlation functions are essential for characterizing the response of quantum many-body systems to external perturbation. As their calculation is classically intractable in general, quantum algorithms are promising in this aspect, but most rely on brute force measurement strategies that evaluate one body observable pair per circuit. In this work, we introduce Fermionic-Adapted Shadow Tomography (FAST) protocols, a new framework for the efficient calculation of multiple dynamical correlation functions. The key idea is to reformulate these functions into forms that are compatible with shadow tomography techniques. The circuits in our protocols require at most two-copy measurements with uncontrolled Hamiltonian simulation. We show that the proposed protocols enhance sample efficiency and/or reduce the number of measurement circuits by one or two orders of magnitude with respect to the system size across a range of scenarios.

Reference: https://arxiv.org/abs/2508.03192

Poster No. 15

Universal Behavior and Its Breakdown in the One-Band Hubbard Model under an Electric Field

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The metal-to-insulator transition (MIT) in the single-orbital Hubbard model has been extensively studied as a function of Coulomb interaction strength and temperature. Near the transition, equilibrium resistivity exhibits universal scaling behavior, collapsing onto distinct metallic and insulating branches. In this work, we investigate whether such universality persists under nonequilibrium conditions. Using the non-crossing approximation, we examine electric-field-driven electronic states in the single-orbital Hubbard model over a range of temperatures. By analyzing the scaling behavior of nonequilibrium transport properties, we assess the robustness of the equilibrium universality in driven correlated systems. Our results provide insight into the critical behavior of field-induced MITs and suggest directions for future studies of nonequilibrium phenomena in strongly correlated materials.

Poster No.16

Toric code under antiferromagnetic isotropic Heisenberg interaction

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We investigate the impact of an isotropic antiferromagnetic Heisenberg perturbation on the toric code, focusing on the resulting quantum phase transition and the nature of the phase that emerges beyond topological order. Using neural-network quantum states, we compute ground states over a wide range of Heisenberg couplings while fully respecting the exact symmetries of the model. In the weak-coupling regime, the numerical results are in excellent agreement with an effective low-energy description derived from a Schrieffer-Wolff (SW) transformation, providing analytic control over the perturbative breakdown of topological order. We show that the Heisenberg perturbation only renormalizes local operators at low orders, whereas mixing between topological sectors occurs only at a perturbative order proportional to the system size. At intermediate values of the Heisenberg interaction, the topological phase breaks down. We estimate the critical point through a combination of the fidelity susceptibility and the logarithmic susceptibility of noncontractible Wilson loops for various system sizes. Furthermore, we utilize the topological entanglement entropy to provide a comprehensive characterization of the phase transition. Beyond the transition, an antiferromagnetic $\pm X/\pm Z$ Néel phase emerges, characterized by a fourfold-degenerate symmetry-broken manifold, which is explicitly probed using staggered-magnetization-based diagnostics. Our results show how local two-spin interactions, which naturally arise in realistic implementations of the toric code, drive the breakdown of topological order. Moreover, we establish the SW approach as a systematic framework for analyzing such perturbations in combination with variational many-body methods.

Development of the Divide-and-Conquer Projected UHF Method for Strongly-Correlated Large-Scale Systems

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The treatment of static electron correlation is still challenging, especially in large systems. In this study, we developed the DC-PUHF method, which combines the divide-and-conquer (DC) method[1] with the projected UHF (PUHF) method[2]. The PUHF method extracts the correct spin state from the UHF wavefunction, which suffers from the spin contamination, by means of a projection operator based on the generator coordinate method and can handle static electron correlations in a black-box manner. First, we applied the DC method to the process of the diagonalization of the projected Fock matrix in the PUHF method[3]. Figure 1 shows the calculated potential energy curve of a polyquinodimethane (n=15) when the terminal benzene ring is rotated, demonstrating the quantitative accuracy of the DC-PUHF method. The time for the projected Fock matrix diagonalizations in the (DC-)PUHF method, shown in Fig. 2, indicates that the DC-PUHF method achieves linear-scaling computational cost in the diagonalization step. We are successively developing DC-PUHF method to accelerate the other time-consuming processes.

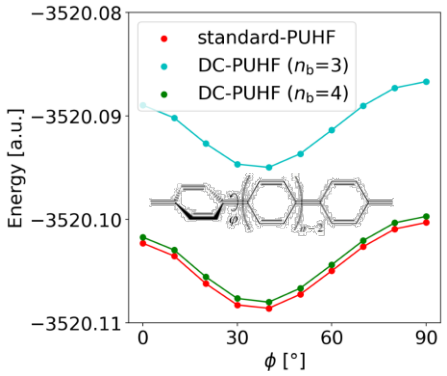

Figure 1: rotational potential energy

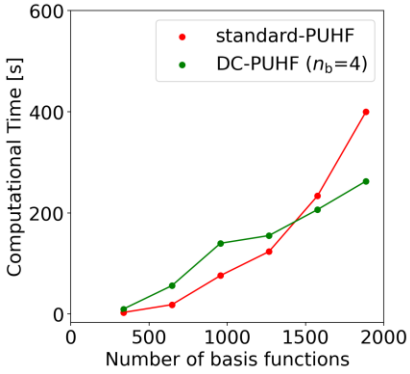

Figure 2: diagonalization scale

[1] H. Nakai *et al.*, *J. Phys. Chem. A* **127**, 589 (2023).
[2] C.A. Jiménez-Hoyos *et al.*, *J. Chem. Phys.* **136**, 164109 (2012).
[3] T. Yoshikawa, S. Kasaya, M. Nishida, T. Taketsugu, and M. Kobayashi, *J. Chem. Theory Comput.*, *in press.*

Poster No.18

Disentangling Haldane phase by Generalized Clifford Circuits

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Disentangling transformations play a central role in the classical simulation of quantum many-body systems, yet their structure remains largely unexplored. Here, we investigate disentangling in spin-1 systems using generalized Clifford circuits, with particular emphasis on the Haldane phase. To this end, we extend the Clifford-circuit-augmented matrix product states (CAMPS)-based density-matrix renormalization group (DMRG) method to spin-1 systems. This leads us to identify the generalized Kramers-Wannier (KW) transformation as an optimal Clifford disentangler for the Haldane phase, and its optimality is analytically verified for the Affleck-Kennedy-Lieb-Tasaki (AKLT) state. More importantly, the disentangling circuits do not merely reduce entanglement, but also expose the physical structure of the underlying phases: the KW transformation maps the Haldane phase onto a phase with spontaneous breaking of a Z_2 symmetry. This correspondence is structurally distinct from the Kennedy-Tasaki transformation, identifying a new unitary route from symmetry-protected topological order to symmetry breaking.

Poster No.19

Pressure-Driven Superconductivity and Emergent Topological Phases in MPX_3 (M=Fe, Ni; X=S, Se)

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The layered magnetic thiophosphates MPX3 (M = Fe, Ni; X = S, Se) host pressure-tunable electronic phases, which we investigate through a systematic first-principles study. Density functional perturbation theory reveals strikingly contrasting superconducting behavior across this family, ranging from conventional phonon-mediated pairing to cases where electron–phonon coupling alone cannot account for the observed superconductivity. We further find that pressure stabilizes nontrivial Z_2 topological phases in the high-pressure P-31m structure, accompanied by symmetry-protected band inversions and surface states. Pressure thus emerges as a unified knob that simultaneously controls magnetism, superconductivity, and topology, making compressed MPX_3 a promising playground for intertwined quantum phenomena.