PROGRAM AND ABSTRACTS

Computational Quantum Many-Body Theory

July 2 – 4, 2025

Rm. 1503, KIAS, Seoul

Plenary Speakers

Evgeny Kozik, King's College London, UK

Gabriel Kotliar, Rutgers University, USA

Synge Todo, The University of Tokyo, Japan

Invited Speakers

Andreas Weichselbaum, Brookhaven National Laboratory, USA

Bongjae Kim, Kyungpook National University, South Korea

Chang-Jong Kang, Chungnam National University, South Korea

Chia-Min Chung, National Sun Yat-sen University, Taiwan

Dong-Hee Kim, Gwangju Institute of Science and Technology, South Korea

Hiroshi Shinaoka, Saitama University, Japan

Hongbin Zhang, Technical University of Darmstadt, Germany

Kun Woo Kim, Chung-Ang University, South Korea

Kyo-Hoon Ahn, Czech Academy of Sciences, Czechia

Sangkook Choi, Korea Institute for Advanced Study, South Korea

Seung-Sup Lee, Seoul National University, South Korea

Thomas Ayral, Eviden Quantum Lab, France

Session Chairs

Heung-Sik Kim, Kangwon University, South Korea

Hunpyo Lee, Kangwon University, South Korea

Hyun-Yong Lee, Korea University, South Korea

Ji Hoon Shim, Postech, South Korea

Myung Joon Han, KAIST, South Korea

Organizing Committee

Aaram J. Kim, DGIST, South Korea

Sangkook Choi, Korea Institute for Advanced Study, South Korea

Seung-Sup B. Lee, Seoul National University, South Korea

Se Young Park, Soongsil University, South Korea

Computational Quantum Many-body Theory

	July 2 (Wed)	July 3 (Thu)	July 4 (Fri)
9:00-9:30	Registration		
9:30-10:30	**Chair: Ji Hoon Shim**	**Chair: Hyun-Yong Lee**	**Chair: Myung Joon Han**
	Gabriel Kotliar	Synge Todo	Evgeny Kozik
10:30-11:10	Chang-Jong Kang	Dong-Hee Kim	Kun Woo Kim
11:10-11:50	Hongbin Zhang	Chia-Min Chung	Hiroshi Shinaoka
11:50-13:30	**Lunch**		
13:30-14:10	**Chair: Hunpyo Lee**	**Excursion and Dinner**	**Chair: Heung-Sik Kim**
	Bongjae Kim		Seung-Sup Lee
14:10-14:50	Thomas Ayral		Kyo-Hoon Ahn
14:50-15:30	Sangkook Choi		Andreas Weichselbaum
15:30-16:00	Coffee Break		
16:00-18:00	**Poster Session**		
18:00-20:00	**Banquet**		

ABSTRACTS OF TALKS

DMFT and g-RISB: some unexpected connections

Gabriel Kotliar

Rutgers University

Quantum embedding methods have revolutionized our understanding of strongly correlated electron materials, and opened the way to compute their physical properties starting from first principles. Traditional auxilliary particle methods, such as the slave boson method preceded DMFT are computationally much faster, but at the same time less accurate than DMFT. Surprisingly, it's possible to formulate them in the language of quantum embedding methods and this new perspective gave rise to new extensions to make their accuracy closer to that of DMFT without increasing too much its computational cost.

We will review some of these developments and illustrate them with both first principles calculations of materials as well as model Hamiltonian studies and conclude with promising future directions.

Electronic structure and physical properties of altermagnetic systems

Chang-Jong Kang

Department of Physics, Chungnam National Unviersity, Daejeon 34134, Republic of Korea

Altermagnetism is a recently identified fundamental form of magnetism characterized by a vanishing net magnetization and a broken electronic structure with time-reversal symmetry. In this talk, we employ a combination of symmetry analysis and first-principle calculations to reveal that the crystallographic symmetry groups of numerous magnetic materials, featuring negligibly small relativistic spin-orbit coupling (SOC), are significantly larger than conventional magnetic groups. Consequently, a symmetry description incorporating partially decoupled spin and spatial rotations, termed the spin group, becomes essential. We establish the classifications of spin point groups that describe collinear magnetic structures, encompassing altermagnetic phases. Using MnTe as an example, we provide direct evidence for altermagnetism in MnTe.

Spectroscopic and energetic features of electronic correlations in functional materials

Hongbin Zhang

Institute of Materials Science, Technical University of Darmstadt, Darmstadt 64287, Germany

Advanced functional materials are of pivotal importance for future sustainable developments of our society, where the rational design of such materials entails profound mechanistic understanding of their physical properties. In this work, taking permanent magnets and battery cathode materials as examples, I am going to showcase how to quantify the corresponding features of correlated electrons. On the one hand, for high-performance permanent magnets comprising 4f rear-earth and 3d transition-metal elements, it is critical to decipher the behavior of 4f electrons driven by the interplay of hierarchical interactions. Correspondingly, I will elaborate how an efficient workflow can be constructed to parameterize DFT results and how to solve the resulting local atomic Hamiltonian to obtain energetic (i.e., magnetic anisotropy) and spectroscopic (e.g., x-ray circular dichroism) features, validated with experimental results. On the other hand, for battery cathode materials based on transition-metal oxides, I am going to demonstrate how x-ray absorption and photoelectron spectroscopies can be evaluated considering both local and long-range charge fluctuations to elucidate on the local structural variations during the (dis-)charging processes. Lastly, combined with machine learning (in particular Bayesian optimization) techniques, it is demonstrated that the local electronic/spin Hamiltonians can be identified in an automatized manner based on the spectroscopic data, enabling not only more efficient sampling for experimental data acquisition but also autonomous characterization/understanding of the underlying correlated physics in the future.

Role of *nonlocal* Coulomb interactions in perovskite transition metal oxides

Bongjae Kim

Kyungpook National University

Employing the density functional theory incorporating on-site and inter-site Coulomb interactions (DFT+*U*+*V*), we have investigated the role of the nonlocal interactions on the electronic structures of the transition metal oxide perovskites. Using constrained random phase approximation (cRPA) calculations, we derived screened Coulomb interaction parameters and revealed a competition between localization and screening effects, which results in nonmonotonic behavior with *d*-orbital occupation. We highlight the significant role and nonlocality of inter-site Coulomb interactions, *V*, comparable in size 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 hybridization between transition metal *d* and oxygen *p* orbitals as occupation increases. We further demonstrate that the inclusion of the inter-site *V* is essential for accurately reproducing the experimental magnetic order in transition metal oxides. If time allows, we will also discuss methodological aspects of the cRPA approach.

S2-2

Quantum computing with and for many-body physics

Thomas Ayral

Eviden Quantum Laboratory, 78340 Les Clayes-sous-Bois, France

The many-body problem is ubiquitous in condensed-matter physics, quantum chemistry and even applied mathematics (where is it known as combinatorial optimization). It represents a very hard computational challenge that is met with sophisticated classical algorithms, which come with limitations in some regimes. On the other hand, a new generation of processors called quantum processors has emerged in the last decade that can manipulate hundreds of quantum bits for thousands of operations. These processors are themselves a many-body problem. In this presentation, I will show that this makes quantum processors a promising tool to accelerate the resolution of many-body problems, but also asks for a careful comparison with classical methods: physical effects like decoherence degrades quantum computations, and classical methods already bring powerful intuitions. I will thus argue that classical methods to reach potential quantum advantage: for instance, tensor networks can be used as benchmarking tools [1] or warm-starters for quantum computations [2], while quantum embedding methods can be used to take advantage of the natural decoherence of quantum computers [3].

[1] Thomas Ayral, Thibaud Louvet, Yiqing Zhou, Cyprien Lambert, E Miles Stoudenmire, Xavier Waintal (2022). A density-matrix renormalisation group algorithm for simulating quantum circuits with a finite fidelity. Physical Review X Quantum 4, 020304.

[2] Baptiste Anselme Martin, Thomas Ayral, François Jamet, Marko Rancic, Pascal Simon (2023). Combining Matrix Product States and Noisy Quantum Computers for Quantum Simulation, Physical Review A, 109, 062437.

[3] Corentin Bertrand, Pauline Besserve, Michel Ferrero, Thomas Ayral (2024). Turning qubit noise into a blessing: Automatic state preparation and long-time dynamics for impurity models on quantum computers, arXiv:2412.13711.

Quantum Zeno Monte Carlo for computing observables

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

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

The recent development of logical quantum processors marks a pivotal transition from the noisy intermediate-scale quantum (NISQ) era to the fault-tolerant quantum computing (FTQC) era. These devices have the potential to address classically challenging problems with polynomial computational time using quantum properties. However, they remain susceptible to noise, necessitating noise resilient algorithms. We introduce Quantum Zeno Monte Carlo (QZMC), a classical-quantum hybrid algorithm that demonstrates resilience to device noise and Trotter errors while showing polynomial computational cost for a gapped system. QZMC computes static and dynamic properties without requiring initial state overlap or variational parameters, offering reduced quantum circuit depth.

[1] M. Han, H. Park, and S. Choi, Quantum Zeno Monte Carlo for computing observables, Npj Quantum Inf **11**, 1 (2025).

Advanced Tensor Network Algorithms for Quantum Many-Body Problems and Quantum Computation

Synge Todo

Department of Physics, The University of Tokyo, Tokyo 113-0033, Japan

Tensor networks offer a powerful and versatile framework for addressing the complexity of quantum many-body systems and the challenges in quantum computing. This talk presents recent advances in applying tensor network algorithms within quantum-classical hybrid computing frameworks, particularly their integration with high-performance computing (HPC) environments. We explore how tensor networks serve as efficient representations for quantum states, enabling breakthroughs in quantum embedding schemes, error correction protocols, and circuit simulation techniques. We further highlight the emerging role of tensor-network-based Monte Carlo methods, which combine the strengths of stochastic sampling and structured representations to enhance simulation accuracy and scalability. Beyond quantum simulation, we discuss the synergy between tensor networks and quantum machine learning, emphasizing their shared mathematical structures and potential for mutual advancement.

Disordered flat-band superconductivity in the kagome Hubbard model

Dong-Hee Kim

Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Korea

We investigate the fate of the flat-band superconductivity in the attractive Hubbard model on the kagome lattices under disorder. We consider two types of disorder: the uncorrelated random onsite potential and the correlated disorder [Phys. Rev. B 98, 235109 (2018)] designed to preserve the flat band in the parent noninteracting Hamiltonian. Using the Bogoliubov-de Gennes mean-field and exact diagonalization calculations, we find that superconductivity is significantly more resilient to the flat-band preserving disorder compared to the uncorrelated random potential. While both cases develop spatial inhomogeneity in the pairing as disorder increases, eventually leading to the superconductor-insulator transition, it turns out that the geometric contribution to the superfluid weight remains robust as long as the flat-band degeneracy is intact. We observe that the flat-band signature in the superfluid weight that is linearly proportional to the interaction strength persists with the flat-band-preserving disorder.

Numerical studies of superconductivity with partially filled stripes in the Hubbard model

Chia-Min Chung

National Sun Yat-sen University

The Hubbard model is an foundational model in quantum many-body physics and has been intensely studied, especially since the discovery of high-temperature cuprate superconductors. The development of advanced numerical techniques, such as tensor networks and quantum Monte Carlo, now enables highly accurate simulations of correlated electron systems. In this talk, I will introduce our works in numerical studies on the two-dimensional Hubbard model. Recently, we found superconductivity in both the electron- and hole-doped regimes of the two-dimensional Hubbard model with next-nearest neighbor hopping. In the electron-doped regime, superconductivity was weaker and was accompanied by antiferromagnetic Néel correlations at low doping. The strong superconductivity on the hole-doped side coexisted with stripe order, which persisted into the overdoped region with weaker hole-density modulation. These stripe orders varied in fillings between 0.6 and 0.8. Our results suggest the applicability of the Hubbard model with next-nearest hopping for describing cuprate high–transition temperature (Tc) superconductivity.

Fast diagrammatic calculations on classical — and possibly quantum — computers

Evgeny Kozik

Department of Physics, King's College London, London, UK

Feynman's diagrammatic series is a common language for a formally exact theoretical description of systems of infinitely-many interacting quantum particles, as well as a foundation for precision computational techniques. I will present a versatile framework for efficient and numerically exact evaluation of diagrammatic expansions of arbitrary structure. It is based on an explicit combinatorial construction of the sum of the integrands of all diagrams by dynamic programming, at a computational cost that can be made only exponential in the diagram order on a classical computer and potentially polynomial on a quantum computer. I will illustrate the technique by its application to controlled solution of correlated systems that remain a challenge for unbiased methods, including the SU(N) Hubbard model in an experimentally relevant regime and electrons in the lowest Landau level exhibiting a fractional quantum Hall state.

Cavity quantum electrodynamics of photonic temporal crystals

Kun Woo Kim

Department of Physics, Chung-Ang University, 06974 Seoul, Republic of Korea

Photonic temporal crystals host a variety of intriguing phenomena, from wave amplification and mixing to exotic band structures, all stemming from the time-periodic modulation of optical properties. While these features have been well described classically, their quantum manifestation has remained elusive. Here, we introduce a quantum electrodynamical model of PTCs that reveals a deeper connection between classical and quantum pictures: the classical momentum gap arises from a localization-delocalization quantum phase transition in a Floquet-photonic synthetic lattice. Leveraging an effective Hamiltonian perspective, we pinpoint the critical momenta and highlight how classical exponential field growth manifests itself as wave-packet acceleration in the quantum synthetic space. Remarkably, when a two-level atom is embedded in such a cavity, its Rabi oscillations undergo irreversible decay to a half-and-half mixed state-a previously unobserved phenomenon driven by photonic delocalization within the momentum gap, even with just a single frequency mode. Our findings establish photonic temporal crystals as versatile platforms for studying nonequilibrium quantum photonics and suggest new avenues for controlling light matter interactions through time domain engineering.

Dimensionality Reduction for Quantum Field Theories

Hiroshi SHINAOKA

Department of Physics, Saitama University

Quantum field theories based on Green's functions have been widely used to solve quantum many-body problems. However, many quantum systems exhibit widely varying energy, time, or length scales, which makes them challenging to treat numerically. In this talk, I present two complementary approaches: the intermediate representation (IR) for imaginary-time propagators [1,2] and the quantics tensor train (QTT) representation [3] for general space-time dependencies.

The IR provides a compact and general basis for representing the imaginary-time and imaginary-frequency dependence of propagators. It is constructed via a singular value decomposition of the analytic continuation kernel [1]. Moreover, sparse grids in the imaginary-time and Matsubara-frequency domains associated with the IR can be constructed [2], enabling efficient and stable transformations between the two domains. These techniques have led to significant acceleration of diagrammatic methods such as the GW approximation [2] and Migdal–Eliashberg theory [4,5]. The IR framework can be easily integrated into existing codes using our open-source libraries: sparse-ir (Python) and SparseIR.jl (Julia) [6]. A full implementation in C and Fortran is currently under development [7].

In contrast, the QTT representation enables compression of more general space-time dependencies, including imaginary-time, real-time, and real-space functions with widely varying scales. Importantly, QTTs support fundamental operations—such as integration, Fourier transforms, and convolution—directly in the compressed domain. The usefulness of QTTs for such operations can be further extended [8] by combining them with tensor-network-based machine learning frameworks, such as Tensor Cross Interpolation (TCI) [9,10]. I will highlight recent applications of these techniques, including solutions to the parquet equations at the two-particle level [11], multiorbital impurity models [12], and simulations of nonequilibrium quantum dynamics [13,14].

[1] H. Shinaoka, J. Otsuki, M. Ohzeki, K. Yoshimi, Phys. Rev. B 96, 035147 (2017).
[2] J. Li, M. Wallerberger, C.-N. Yeh, N. Chikano, E. Gull, H. Shinaoka, Phys. Rev. B 101, 035144 (2020).

[3] H. Shinaoka, M. Wallerberger, Y. Murakami, K. Nogaki, R. Sakurai, P. Werner, A. Kauch, Phys. Rev. X 13, 021015 (2023).
[4] T. Wang, T. Nomoto, Y. Nomura, H. Shinaoka, J. Otsuki, T. Koretsune, R. Arita, Phys. Rev. B 102, 134503 (2020).
[5] H. Mori, T. Nomoto, R. Arita, E. R. Margine, Phys. Rev. B 110, 064505 (2024).
[6] M. Wallerberger et al., SoftwareX 21, 101266 (2023).
[7] https://github.com/SpM-lab/libsparseir
[8] M. K. Ritter, Y. Núñez-Fernández, M. Wallerberger, J. von Delft, H. Shinaoka, X. Waintal, Phys. Rev. Lett. 132, 056501 (2024).
[9] Y. Núñez-Fernández, M. Jeannin, P. T. Dumitrescu, T. Kloss, J. Kaye, O. Parcollet, X. Waintal, Phys. Rev. X 12, 041018 (2022).
[10] Y. Núñez-Fernández, M. K. Ritter, M. Jeannin, J.-W. Li, T. Kloss, T. Louvet, S. Terasaki, O. Parcollet, J. von Delft, H. Shinaoka, X. Waintal, SciPost Phys. 18, 104 (2025).
[11] S. Rohshap, M. K. Ritter, H. Shinaoka, J. von Delft, M. Wallerberger, A. Kauch, Phys. Rev. Research 7, 023087 (2025).
[12] H. Ishida, N. Okada, S. Hoshino, H. Shinaoka, arXiv:2405.06440v2 (to appear in PRL).
[13] M. Murray, H. Shinaoka, P. Werner, Phys. Rev. B 109, 165135 (2024).
[14] M. Środa, K. Inayoshi, H. Shinaoka, P. Werner, arXiv:2412.14032.

Hundness in twisted bilayer graphene: correlated gaps and quantum criticalities

Seung-Sup B. Lee

Department of Physics and Astronomy, Seoul National University, Korea

We characterize gap-opening mechanisms and quantum criticalities in the topological heavy fermion (THF) model of magic-angle twisted bilayer graphene (MATBG), with and without electron-phonon coupling, using dynamical mean-field theory (DMFT) with the numerical renormalization group (NRG) impurity solver. In the presence of symmetry breaking associated with valley-orbital ordering (time-reversal-symmetric or Kramers intervalley coherent, or valley polarized), spin anti-Hund and orbital-angular-momentum Hund couplings, induced by the dynamical Jahn–Teller effect, result in a robust pseudogap at filling $2 \lesssim |\nu| \lesssim 2.5$. We identify quantum critical points near the boundaries of the pseudogap regions, which are of Berezinskii–Kosterlitz–Thouless (BKT) or heavy-fermion type, depending on the strengths of the effective Hund couplings determined by the valley-orbital ordering. The pairing susceptibilities are enhanced near these quantum critical points, which might be a precursor to the superconducting phases neighboring $|\nu| = 2$.

Exchange interactions and spin waves in double-layered antiferromagnets: semiclassical model and *ab initio* analysis

Kyo-Hoon Ahn

Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czechia

Traditional approaches to understanding the sign of exchange interactions rely on competition between antiferromagnetic (AFM) and ferromagnetic (FM) contributions by means of wavefunction overlap [1], electrostatic interactions [2], and orbital symmetries [3]. However, these analyses have primarily focused on pairs of actual ions, whereas a comparable study on elementary spins in chain models remains unexplored. This raises a key question: Does such a sign change in exchange parameters apply to pairs of elementary spins, or are there unknown constraints that might control it?

To address this issue, we introduce a novel semiclassical model of magnons in double-layered AFM chains with a collinear ↑↑↓↓ spin order. We underline that conventional FM and AFM chains contain only parallel or antiparallel spin pairs, respectively. In contrast, our model involves both types of pairs at each site, making it a minimal yet ideal framework for exploring the interplay between intra- and inter-sublattice couplings. We find that the surrounding spin configurations can control the sign of exchange parameters and even lead to an AFM sign for the intra-sublattice interactions in our model of railroad trestle (RT) geometry.

We substantiate our findings through direct calculations of the magnon dispersion relation and *ab initio* investigations on AFM CrN. We identify CrN as a unique example where a fully three-dimensional system can be effectively described by a one-dimensional model (RT). This successful application arises from the dominant target ↑↑↓↓ order, which exists exclusively along a single crystallographic direction in double-layered antiferromagnets.

[1] J. C. Slater, Phys. Rev. **36**, 57 (1930).
[2] C. Zener, Phys. Rev. **81**, 440 (1951); Phys. Rev. **83**, 299 (1951).
[3] Y. O. Kvashnin, R. Cardias, A. Szilva, I. Di Marco, M. I. Katsnelson, A. I. Lichtenstein, L. Nordström, A. B. Klautau, and O. Eriksson, Phys. Rev. Lett. **116**, 217202 (2016).
[Preprint] Seo-Jin Kim, Zdeněk Jirák, Jiří Hejtmánek, Karel Knížek, Helge Rosner, and Kyo-Hoon Ahn, arXiv:2412.04685.

Automated Fermionic signs in tensor networks via Z2 graded tensors.

Andreas Weichselbaum

Brookhaven National Laboratory, Upton, NY, USA

It is well known that Fermionic signs in one-dimensional (1D) systems can be taken care of by a Jordan-Wigner transformation. In 2D lattice models, the fermionic projected entangled pair state (fPEPS) construction by Corboz et al. (PRB 2010) has shown that fermionic signs beyond 1D systems can also be treated efficiently locally, albeit with organizational overhead to properly include fermionic parity. More recently it was argued (Mortier et al, SciPost 2024; Gao et al., quant-ph/2024) that fermionic signs can be treated automatically in the tensor framework via Z2-graded tensors. I will briefly review this setting, together with the current status of its implementation in the QSpace tensor library.

ABSTRACTS OF POSTERS

Poster No. 1

Strongly correlated electrons under external bias at steady state

Florian Brette, Gyumin Lee, Geunsik Lee

Department of Chemistry, Center for Superfonctional Materials, Ulsan National Institute of Science and Technology (UNIST), Republic of Korea

We study the steady-state properties of a two-dimensional lattice of strongly correlated electrons using inhomogeneous cluster dynamical mean-field theory (cDMFT). The system consists of a 10×10 array of 2×2 plaquette clusters (4 sites each), with periodic boundary conditions in the transverse direction. A longitudinal bias is applied by connecting the left and right edges to electronic reservoirs with fixed chemical potentials. Each cluster is embedded in a self-consistent bath and solved using exact diagonalization with eight bath sites per impurity. Also, linear and non-linear variations of the chemical potential are considered for different types of local thermalization.

For moderate interaction strength (U = 5.5), the system converges toward a metallic state even at zero bias, despite being initialized from an insulating self-energy obtained from a separate homogeneous DMFT calculation. At slightly stronger interaction (U = 5.7), we observe spatial inhomogeneity in the converged solutions: some clusters remain insulating while others become metallic. In particular, insulating behavior can persist along entire rows or columns over many iterations before giving way to metallicity, or in some cases revert back to insulating. This behavior emerges spontaneously from a spatially uniform initial state and reflects the nonlinear feedback of the self-consistent DMFT loop. When the bias is zero, the cluster momentum components $(\pi,0)$ and $(0,\pi)$ remain degenerate, whereas under finite bias, they evolve differently, indicating symmetry breaking driven by the external field.

These results demonstrate that near the Mott transition, steady-state cDMFT can exhibit domain-like coexistence of metallic and insulating behavior, even in the absence of explicit disorder or symmetry-breaking fields. The findings underscore the sensitivity of correlated systems to both interactions and external driving, and the importance of spatial resolution in capturing real-space electronic phase behavior.

Poster No. 2

Altermagnetism in orthorhombic $NaOsO_3$

Hong-Suk Choi[1], Kyo-Hoon Ahn[2], and Kwan-Woo Lee[1,3]

[1]*Department of Applied Physics, Graduate School, Korea University, Sejong 30019, Korea*
[2] *Institute of Physics, Czech Academy of Sciences, Cukrovarnick´a 10, 162 00 Praha 6, Czechia*
[3]*Division of Semiconductor Physics, Korea University, Sejong 30019, Korea*

Altermagnetism (AM) is a newly identified magnetic phase characterized by spin-split electronic bands, despite having a zero net magnetic moment. This arises since its magnetic sublattices are related by rotational symmetry, in contrast to conventional antiferromagnets, where sublattices are typically connected by translational or inversion symmetry. Interestingly, AM enables spin-dependent transport and gives rise to unconventional forms of the anomalous Hall and spin Hall effects, even in the absence of net magnetization.

In this work, we investigate the orthorhombic perovskite antiferromagnet $NaOsO_3$, which exhibits a high Néel temperature above 410 K and a narrow gap of approximately 70 meV, using *ab initio* calculations. This system has been proposed as the first example of a Slater metal-insulator transition (MIT), in which antiferromagnetic ordering drives the gap opening without any accompanying structural distortion. Consistent with the Slater picture, its most physical quantities evolve continuously across the MIT. However, a discontinuity emerges in the magnetic susceptibility, along with the appearance of a weak magnetic moment of $0.005\mu_B$ at low temperatures.

Through a comprehensive symmetry analysis of the magnetic space group and detailed *ab initio* calculations, we identify the origin of this weak magnetism. Additionally, our results also reveal characteristic signatures of AM in both spin dynamics and transport properties. In the magnon spectra, we observe chiral splittings in both the acoustic and optical branches. Furthermore, the anomalous Hall conductivity exhibits a relatively large magnitude near the Fermi energy. In this presentation, we will discuss these findings in detail.

[Acknowledgements] We acknowledge W. E. Pickett and Myung-Chul Jung for collaborations of this research that is supported by National Research Foundation of Korea (NRF) grants (RS-2024-00392493)

Poster No. 3

Strange diffusivity in half-filled two-dimensional Hubbard model

Youngmin Eom,[1] Igor S. Tupitsyn,[2] Nikolay V. Prokof'ev,[2] Boris Svistunov,[2] Evgeny Kozik,[3] and Aaram J. Kim[1]

[1]*Department of Physics and Chemistry, DGIST, Daegu 42988, Korea*
[2]*Department of Physics, University of Massachusetts, Amherst, Massachusetts 01003, USA*
[3]*Department of Physics, Kings College London, Strand, London WC2R 2LS, United Kingdom*

We study the incoherent charge transport in the half-filled two-dimensional Hubbard model via Nernst–Einstein relation. From the numerically exact results of the dynamic current–current correlation function obtained by the diagrammatic Monte Carlo method which directly access to the thermodynamic limit, we perform the analytic continuation for the optical conductivity using the stochastic optimization method (SOM). The reliability of the SOM results compensated by other numerical analytic continuation methods and the approximate estimations which directly accessible from the Matsubara correlation function. Our analysis reveals an unconventional $1/\sqrt{T}$ dependence of the diffusion constant over a wide range of temperatures and interaction strength, where the DC resistivity exhibits anomalous T or $\sqrt{T}$ scaling. This behavior is intriguingly consistent with recent cold-atom lattice experiments on doped systems [1]. Furthermore, by distinguishing the bubble and vertex diagrams in the optical conductivity, we demonstrate that the bubble term predominantly governs incoherent transport in high temperatures while the vertex correction becomes significant only near the metal-to-insulator crossover regime.

[1] Brown, P. T., Mitra, D., Guardado-Sanchez, E., Nourafkan, R., Reymbaut, A., Hébert, C. D., ... & Bakr, W. S. (2019). Science, 363(6425), 379-382.

Poster No. 4

Solving the nonequilibrium Dyson equation with quantics tensor trains

Ken Inayoshi[1], Maksymilian Środa[2], Anna Kauch[3], Philipp Werner[2], and Hiroshi Shinaoka[1]

[1]Department of Physics, Saitama University, [2]Department of Physics, University of Fribourg, [3]Institute of Solid State Physics, TU Wien

Nonequilibrium correlated electron systems exhibit a wide variety of physical phenomena across different time scales. Numerical studies of these phenomena require the accurate descriptions of short- to long-time dynamics. The nonequilibrium Green's function (NEGF) method [1,2] is a powerful tool for treating electron correlations and time-evolution on equal footing. However, in nonequilibrium systems, the Green's function depends on two-time variables. This leads to a significant increase of memory usage, especially in long-time simulations.

To address this challenge, various memory compression techniques [3,4,5] have been proposed for the NEGF method. Among them, a tensor network approach known as the quantics tensor train (QTT) has attracted attention for its ability to exponentially compress the data size of Green's functions [6]. Although a prototype implementation of NEGF methods with QTT has been developed, its benchmarks have been limited to short-time simulations because of technical difficulties, such as the slow convergence of self-consistent calculations [7].

To enable simulations over longer timescales, we propose an improved implementation. We introduce a variational linear equation solver for the Dyson equation [8], and a divide-and-conquer algorithm that exploits the causality of Green's functions [9]. In this talk, we benchmark our methods using relevant test cases [8,9].

[1] H. Aoki *et al.*, Rev. Mod. Phys. **86**, 779 (2014).
[2] M. Schüler *et al.*, Compt. Phys. Comm. **257**, 107484 (2020).
[3] P. Lipavský *et al.*, Phys. Rev. B **34**, 6933 (1986).

[4] M. Schüler *et al.*, Phys. Rev. B **97**, 245129 (2018).
[5] J. Kaye and D. Golež, SciPost Phys. **10**, 091 (2021).
[6] H. Shinaoka *et al.*, Phys. Rev. X **13**, 021015 (2023).
[7] M. Murray, H. Shinaoka, and P. Werner, Phys, Rev. B **109**, 165135 (2024).
[8] M. Środa, K. Inayoshi, H. Shinaoka, and P. Werner, arXiv: 2412.14032.
[9] K. Inayoshi, M. Środa, A. Kauch, P. Werner, and H. Shinaoka, in preparation.

Poster No. 5

Examining Magnetic Properties and Multiferroicity in the Isostructural Cu_2TSiS_4 (T = Mn and Fe) System

Jo JongIn

POSTECH, chemistry

The stannite-type Cu_2TSiS_4 (T = Mn and Fe) compounds are promising multifunctional materials due to their noncentrosymmetric crystal structure, which enables magnetic ordering, ferroelectricity, and nonlinear optical activity. Despite structural similarities, Cu_2MnSiS_4 and Cu_2FeSiS_4 exhibit distinct antiferromagnetic (AFM) orderings characterized by propagation vectors k = (½ , 0, ½) and (½ , ½ , ½), respectively.

To uncover the origin of this contrast, we performed density functional theory (DFT + U) calculations combined with orbital interaction analysis. We find that the J_5 spin exchange, which runs along the *b*-axis, is critical in determining the magnetic ordering difference. Notably, the participation of the Cu^+ ion, through its 4s orbital, breaks the orthogonality of S 3p orbitals and induces AFM coupling in J_5. This Cu-mediated effect is stronger in Cu_2FeSiS_4 due to its shorter Cu–S bond length and larger S–Cu–T angle.

We further evaluated the ferroelectric (FE) polarization using DFT + U and DFT + U + SOC methods. The results show that both materials exhibit robust FE polarization along the *c*-axis, primarily arising from their noncentrosymmetric structure, rather than from magnetic ordering or spin–orbit coupling.

Our findings demonstrate how subtle orbital interactions, especially involving nominally non-magnetic Cu^+ ions, can significantly influence magnetic ground states in structurally similar compounds, offering insights for designing multiferroic and spintronic materials.

Poster No. 6

Global phase diagrams of the two-spin-orbital Kondo models with and without orbital exchange anisotropy

Hyunsung Jung[1,2], Sanghyun Park[1,2], and Seung-Sup Lee[1,2,3]

[1]*Department 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*

Hundness in two-orbital (e_g) systems has gained recent interest as a potential mechanism for strong correlations in Ni-based materials. In the context of dynamical mean-field theory (DMFT) studies of Hund metals, the non-Fermi liquid (NFL) behaviors are characterized by studying the spin-orbital Kondo impurity models as effective models of the original lattice systems. While the three-spin-orbital Kondo model for t_2g systems is better understood, its two-spin-orbital counterpart for e_g systems is less scrutinized. In this work, we investigate the two-spin-orbital Kondo models with and without orbital exchange anisotropy using the numerical renormalization group (NRG) method. In the isotropic case, we identify three NFL phases (i) with decoupled spin and overscreened orbital degrees of freedom; (ii) with decoupled orbital and overscreened spin; and (iii) with both spin and orbital overscreened. Anisotropic orbital exchange can further induce (iv) another NFL phase where the orbital degrees of freedom become ferromagnetic while spin is overscreened. We also find that the transition between phases (iii) and (iv) is of the Berezinskii–Kosterlitz–Thouless (BKT) type.

Poster No. 7

Clebsch–Gordan coefficients without floating-point error: toward a non-Abelian-symmetric tensor library

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

[1]*Department 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*

Tensor libraries that exploit non-Abelian symmetries decompose tensors using the Wigner–Eckart theorem for more efficient storage and manipulation of tensors. However, the numerical treatment of the Clebsch–Gordan coefficients (CGCs) is susceptible to floating-point error, especially for large multiplets. Here, we develop a new algorithm for generating and manipulating CGCs exactly, which uses integer operations only and takes advantage of the structure of the Lie algebra for further efficiency. Our Julia implementation generates SU(2) CGCs about 10 times faster than QSpace, the state-of-the-art tensor library. The algorithm will be used as the core of a fast, accurate, and scalable non-Abelian-symmetric tensor library.

Poster No. 8

Classical optimization algorithms for diagonalizing quantum Hamiltonians

Taehee Ko[1], Hyowon Park[2], Sangkook Choi[1], Xiantao Li[3]

1. *Computational Sciences, Korea Institute for Advanced Study*
2. *Department of Phyiscs, University of Illinois at Chicago*
3. *Department of Mathematics, the Pennsylvania State University*

Diagonalizing a Hamiltonian has recently gained increasing attention for practical circuit synthesis in quantum computing applications such as Hamiltonian simulation. As it is not possible in general, of significant importance is the task of identifying Hamiltonians for which, once diagonalized, a fixed, polynomially sized quantum circuit can implement arbitrarily long-time simulations, enabling fast-forwarding and highly accurate energy estimation. Despite these practical implications, only a few diagonalization algorithms exist with a few families of such Hamiltonians known, and some incur classical costs that exceed the cubic scaling of conventional eigensolvers. In this work, we introduce new classical optimization algorithms for Hamiltonian diagonalization by formulating a cost function that penalizes off-diagonal terms and enforces unitarity via an orthogonality constraint, both expressed in the Pauli operator basis. While theoretically similar or equivalent to existing Lie-algebraic methods in special cases, our approach applies more generally and significantly streamlines the iterative process. We prove that the optimization landscape admits only nonzero global minima corresponding to valid diagonalizations (aside from the trivial zero solution), and we establish convergence of the deterministic algorithm under a mild nonconvexity condition validated numerically. Furthermore, we propose a randomized-coordinate variant that achieves quadratic per-iteration cost scaling in the Hilbert-space dimension, an order of magnitude improvement over prior techniques. Importantly, we identify a new class of Hamiltonians for which existing Lie-diagonalization methods incur exponential per-iteration costs, whereas our algorithm remains polynomially efficient. Finally, we demonstrate these advantages through explicit examples and numerical experiments.

Poster No. 9

Scalable projected entangled-pair state representation of random quantum circuit states

Sung-Bin B. Lee[1], Hee Ryang Choi[2], Daniel Donghyon Ohm[1], and Seung-Sup B. Lee[1,3,4]

[1]*Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea*
[2]*Department of Mechanical Engineering, Seoul National University, Seoul 08826, Korea*
[3]*Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea*
[4]*Institute for Data Innovation in Science, Seoul National University, Seoul 08826, Korea*

We demonstrate that the simple update method for projected entangled-pair states (PEPS) in the Vidal gauge enables efficient representation of random quantum circuit (RQC) states. Applied to square lattice quantum circuits, the PEPS representation is exact for logarithmic-depth RQCs with polynomial time complexity, surpassing the matrix product state representation. We reveal universal scaling behaviors in the state fidelity by treating large-scale RQCs with up to 10,000 qubits using a single conventional CPU. The fidelity provides the lower and upper bounds of the total-variation distance (error measure based on bitstring probabilities) according to the Fuchs–van de Graaf inequality, where approximate PEPS contraction induces extra error to the total-variation distance.

Poster No. 10

Degeneracy-engineered zero-temperature Mott transition in two-orbital Hund systems

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

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

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 due to 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-Hund model using the state-of-the-art numerical renormalization group (NRG) as a DMFT impurity solver. We demonstrate that the local multiple ground degeneracy ($D_{g)}$ is crucial; the transition is first-order as long as D_g is less than the number of orbitals plus one, whereas it becomes second-order when D_g equals or exceeds the number of orbitals. Also, we reveal the properties of unstable solutions of first-order transition in two-orbital systems and relate them to those of the one-band Hubbard model at finite temperature.

[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. 11

Role of electron-phonon coupling and symmetry breaking in dynamic correlations in twisted bilayer graphene

Seongyeon Youn[1,2*], Beomjoon Goh[1,2,3*], Geng-Dong Zhou[4], Zhi-Da Song[4,5,6†], and Seung-Sup B. Lee[1,2,3†]

Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea
Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea
Institute for Data Innovation in Science, Seoul National University, Seoul 08826, Korea
International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China
Hefei National Laboratory, Hefei 230088, China
Collaborative Innovation Center of Quantum Matter, Beijing 100871, China

We study the topological heavy fermion (THF) model of magic-angle twisted bilayer graphene (MATBG), with and without electron-phonon coupling, using dynamical mean-field theory (DMFT) with the numerical renormalization group (NRG) impurity solver. In the presence of symmetry breaking associated with valley-orbital ordering (time-reversal symmetric or Kramers intervalley coherent, or valley polarized), we observe that spin anti-Hund and orbital-angular momentum Hund couplings, induced by the dynamical Jahn–Teller effect, lead to (i) a robust pseudogap within the filling range $2 \lesssim |\nu| \lesssim 2.5$, and (ii) quantum critical points at fractional fillings $|\nu| \approx 1.6$ and $|\nu| \approx 2.7$. Regimes near these critical points coincide with both the region where pairing susceptibilities are significantly enhanced and the experimentally observed superconducting dome. In this respect, we suggest that these quantum criticalities are related to the superconductivity in MATBG.

Poster No.12

Overlap guided constant speed scheduling for the quantum adiabatic evolution

Mancheon Han[1], Hyowon Park[2,3], SangKook Choi[1]

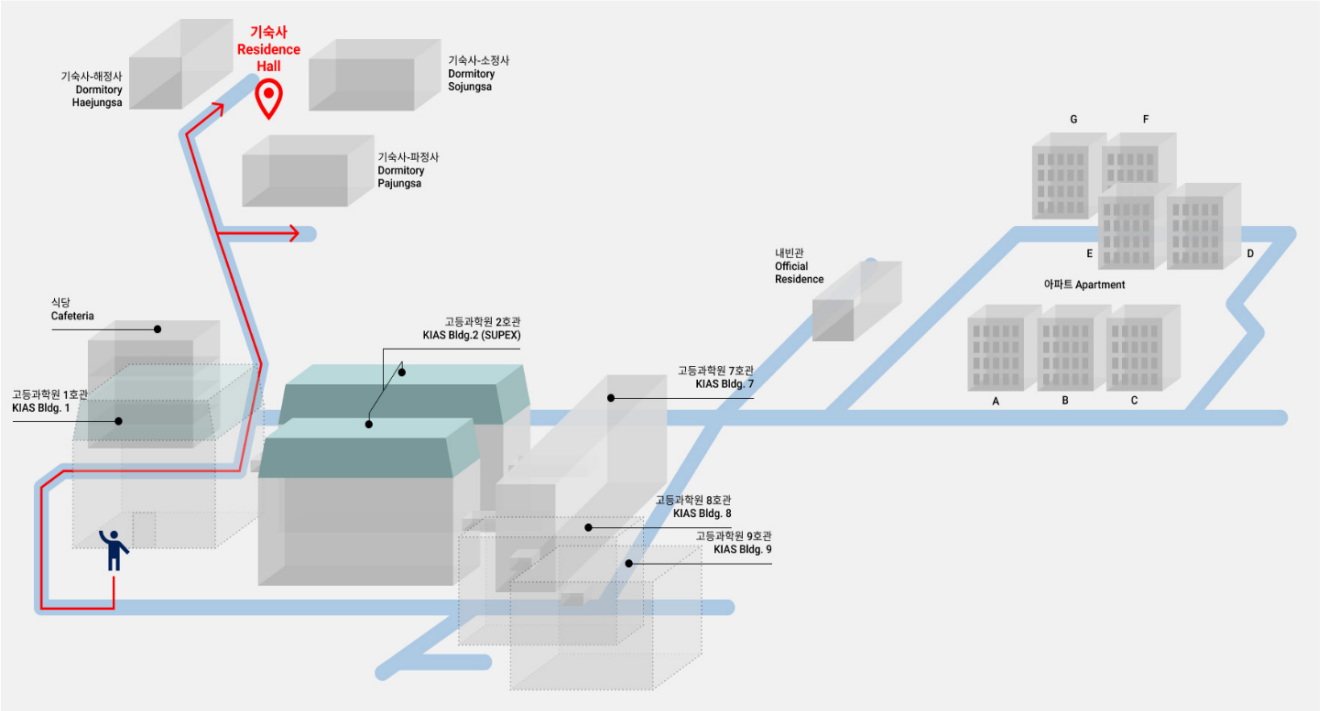
[1]*Department of Computational Sciences, Korea Institute for Advanced Study (KIAS),*

[2]*Materials Science Division, Argonne National Laboratory,*

[3]*Department of Physics, University of Illinois at Chicago*

The adiabatic theorem, first formulated by Born and Fock in 1928, asserts that a quantum system remains in its instantaneous eigenstate if perturbations vary slowly enough. This principle underpins quantum phase classification and quantum computation. While gradual interpolation between an initial Hamiltonian and a target Hamiltonian ensures convergence, performance depends critically on the schedule function. We introduce overlap-guided constant-speed scheduling, which evaluates eigenstate overlaps to segment the adiabatic path and maintain uniform evolution speed. Using this schedule, we show that the gap dependence of the required evolution time improves by one order in the energy gap, which is particularly beneficial for small-gap systems. We also propose a practical algorithm based on the Quantum Zeno Monte Carlo (QZMC) method to estimate overlaps. Numerical simulations on adiabatic Grover search, the N_2 molecule, and an iron–sulfur complex confirm that our approach reduces runtime scaling with the energy gap, yielding significant speedups.

Bldg.1 to Residence Hall



Transportation

Bus – 201, 273

- Get off at 'KAIST /Hong-neung Elementary School'.

Metro – line no.1

- Get off at 'Cheongnyangni' or 'Hoegi' Station.

From Hoegi Station

1. From exit No. 1, turn left and follow the sidewalk on the right until you reach the intersection and crosswalk.
2. Cross the street and turn right.
3. Go straight until you see the bus stop.
4. Take No.273 and get off at 'KAIST /Hong-neung Elementary School'.

From Cheongnyangni Station

1. When you get out through exit No. 2, ignore the bus stop you see right away and follow the way without making turns until you see another bus stop.
2. Take No. 201 and get off at 'Hong-neung Elementary School' bus stop.
3. You will see KIAS(KAIST campus) across the street.