Chapter 9

Computational Materials Science Research Team

9.1 Members

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9.2 Overview of Research Activities

Strongly correlated quantum materials show great promise for next-generation electronic applications. In order to accelerate the development of functional strongly correlated quantum materials, a reliable theory with good predictability is required. However, the strong interactions that take place in this class of materials do not allow us to apply the traditional band theory based on the density functional theory, which played a major role in the advance of today's electronic technology based on semiconductors.

Consequently, we are developing large-scale numerical simulations for strongly correlated quantum systems, including strongly correlated quantum materials, where the many-body interactions are essential to induce novel phenomena and properties. We are interested particularly in the quantum Monte Carlo (QMC) method, the density matrix renormalization group (DMRG) method, and the tensor network method to simulate not only the ground state but also the dynamics (thermodynamics, excitation dynamics, and real time dynamics). We have established a platform for advanced research of strongly correlated quantum systems by developing state-of-the-art simulations.

9.3 Research Results and Achievements

9.3.1 Large-scale QMC simulations for interacting fermions

We develop a quantum Monte Carlo (QMC) method, which is one of the most reliable and efficient techniques for Hubbard-type lattice models of interacting electrons. Typical target systems we aim are of the order of 10,000 electrons unless the notorious minus-sign problem occurs. One of the main focuses in our QMC project is to clarify quantum criticality of quantum phase transitions in strongly-correlated electrons with high accuracy, which would be impossible without the power of super computers.

We have implemented a highly efficient QMC code based on the auxiliary field scheme for lattice fermion systems at zero temperature. Since numerical calculations involved in this formulation are mostly linear algebraic procedure such as matrix-matrix product and numerical orthogonalization, we can take advantage of the highly optimized numerical library on super computers such as K computer to calculate physical observables with a high degree of accuracy on unprecedentedly large systems.

In this fiscal year, we have revisited the quantum criticality of the phase transitions for the chiral-Heisenberg universality class in terms of the Gross-Neveu model. The linear dispersion of the Dirac fermions in the non-interacting limit, as shown in Fig. 9.1, is constructed by introducing a d-wave pairing field to the Hubbard model on the square lattice. The Hamiltonian we have studied reads

$$H = H_{\mathrm{BCS}} + H_U, \tag{9.1}$$

where

$$H_{\mathrm{BCS}} = \sum_{\langle i,j \rangle} \left\{ \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow} \end{pmatrix} \begin{pmatrix} -t & \Delta_{ij} \\ \Delta_{ij}^* & t \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}^\dagger \end{pmatrix} + \mathrm{h.c} \right\} \tag{9.2}$$

and

$$H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{9.3}$$

It is noted that, the way of counting the number of fermion components being different, the effective model in the continuum limit is the same as that of the widely-studied Hubbard model on the honeycomb lattice, of which the critical exponents have been accurately determined in our previous study.

By exploiting large-scale quantum Monte Carlo simulations, we have calculated the correlation ratio of the spin structure factor, the staggered magnetization, and the quasiparticle weight. Based on these quantities, the antiferromagnetic phase transitions have been investigated by several methods such as the crossing-point analysis (Fig. 9.2) and the data-collapse fit (Fig. 9.3). The conservative estimates for the critical exponents obtained in this work are ν=1.05(5), η_ϕ=0.75(4), and η_ψ=0.23(4). These results improve our previous estimates, especially for the exponent η_ϕ, which is now closer to the recent independent QMC calculation which features a quantum spin-Hall insulator transition [Nat. Commun. 10, 1 (2019)]. Indeed we have noticed that it is a cumbersome task to judge whether correction terms to the simple scaling ansatz should be included in a data-collapse fit of the Bayesian scaling analysis, and our previous estimates of η_ϕ were eventually not accurate enough. We have also shown that the anisotropy of the Dirac cones does not affect the criticality, which suggests the emergent relativistic invariance at the quantum critical point.

9.3.2 Massively parallel DMRG algorithms for quantum many-body systems

The DMRG method is recognized as one of the most efficient numerical methods to investigate strongly correlated quantum systems. We have been developing four types of massively parallel DMRG programs, 2D-DMRG, DDMRG, paraDMRG, and QUARTZ. The 2D-DMRG is developed for the ground state calculations on two-dimensional strongly correlated quantum systems. The DDMRG is developed for quantum dynamics of strongly correlated quantum systems. The paraDMRG is developed for the full-CI calculations in *ab initio* simulations. The QUARTZ is developed to simulate quantum computers. Our developed massively parallel DMRG algorithm has achieved the extremely high peak performance ratio of 73.6% when 82,488 nodes are used on K computer, which is about 7.8 PFLOPS.

In this fiscal year, we have developed a new method using supervised machine learning (ML) and DMRG methods to construct phase diagrams in strongly correlated quantum systems. We usually find phase boundaries by detecting anomalous behaviors of physical quantities such as energy. However, these quantities sometimes exhibit little changes at the boundaries. Entanglement spectrum (ES) consisting of the eigenvalues of the entanglement Hamiltonian for the ground state has been suggested as an order parameter. For example, the absence

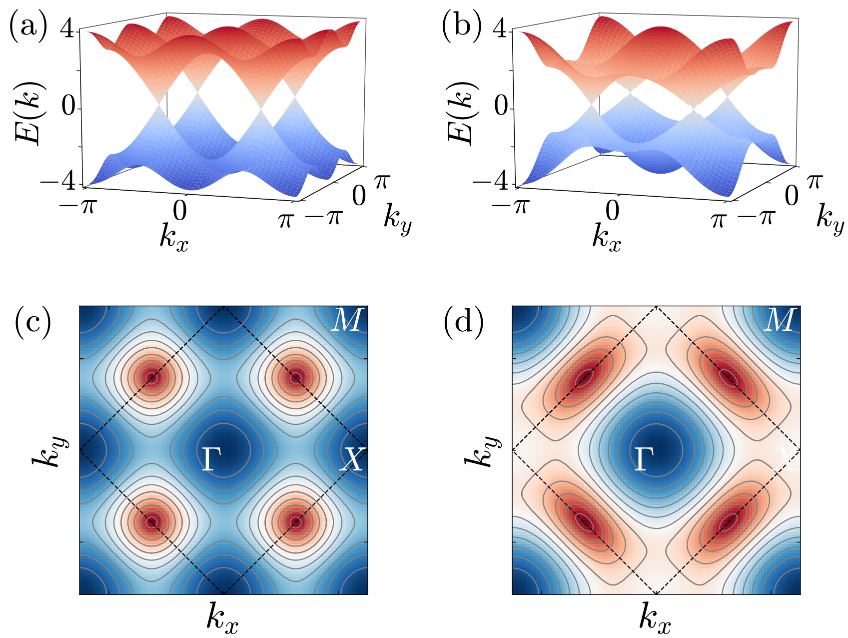

Figure 9.1: The noninteracting energy dispersion of the square lattice Hubbard model with the d-wave pairing field for (a) $\Delta = 1$ and (b) $\Delta = 0.5$, and the corresponding contour plot of the lower band for (c) $\Delta = 1$ and (d) $\Delta = 0.5$.

of a gap called Schmidt gap between the low-lying neighboring two levels of ES is characteristic of topologically ordered phase like the Haldane phase and Kitaev spin liquid phase. Especially, characterizing quantum states by using ES is useful in the DMRG calculations, since ES is always derived in the DMRG procedure. However, the Schmidt gap is not necessarily a good quantity for detecting phase transition between non-topological phases. Another strategy will be the use of ML. In fact, ML has been successful in characterizing ordered states, topological states, and photoexcited states. In the present study, we have used ES as a training dataset of neural network. We have demonstrated that the trained neural network can determine phase boundaries in the half-filled one-dimensional extended Hubbard model.

9.3.3 Controlled dynamics in quantum many-body systems

The recent extensive studies of photoinduced states of strongly correlated quantum systems have paved the way to find new states of matter. Indeed, those activities have found many intriguing phenomena, including the photoinduced transient superconducting states and the photoinduced insulator-to-metal transitions.

Motivated by these experimental activities, we have studied the photoinduced states in models of strongly correlated electron systems. Applying the exact diagonalization technique and the DMRG method, we have found that the pulse irradiation to the Mott insulating state in the Hubbard model can induce the enhancement of an unconventional superconductivity. This photoinduced superconductivity is due to the sequential generation of η-pairs, which is characterized by staggered pair-density-wave oscillations in the off-diagonal long-range correlation with a phase of π (see Fig. 9.4) and is associated with the transverse components of pseudospin $1/2$ operators, first introduced by mathematical physicist C. N. Yang. We have also found that the η pairs are preferentially excited by the optical pulse field because of the beautiful mathematical structure forced by the symmetry of the pseudospin operators.

In our subsequent our works, we have also shown that the same mechanism can be applied to another class of models, the Kondo lattice model, known as an effective model to describe electronic states in heavy electron systems, potentially suggesting that this mechanism can be found ubiquitously. In addition, we have found that the spin dynamics changes drastically and becomes diffusive after pulse irradiation, which can be understood because the generation of the η pairs is equivalent to in-situ carrier doping for spin dynamics.

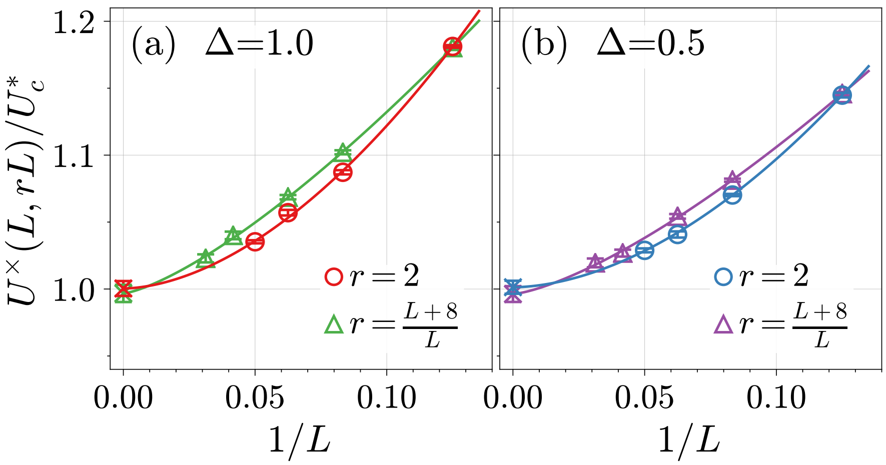

Figure 9.2: Crossing-point analysis of the correlation ratio $R_{m^2}(U, L)$. $U^{\times}(L, rL)$ are obtained by interpolating data points of $R_{m^2}(U, L)$ with second order polynomial functions. For ease of comparison, values of $U^{\times}(L, rL)$ are normalized by $U_{\mathrm{c}}^* = 7.63$ and 5.49 for (a) $\Delta = 1$ and (b) $\Delta = 0.5$, respectively. Ratios of two system sizes are $r = 2$ (circles) and $r = (L + 8)/L$ (triangles). Results of the fit with $U^{\times}(L, rL) = U_{\mathrm{c}} + dL^{-(\omega+1/\nu)}$ are (a) U_{c}=7.63(4) and $\omega + 1/\nu$=1.8(1) for $r = 2$ and U_{c}=7.61(5) and $\omega + 1/\nu$=1.4(1) for $r = (L + 8)/L$, and (b) U_{c}=5.49(3) and $\omega + 1/\nu$=1.8(1) for $r = 2$ and U_{c}=5.47(3) and $\omega + 1/\nu$=1.4(1) for $r = (L + 8)/L$. Note that U_{c}'s extrapolated in the thermodynamic limit are indicated by crosses at $1/L = 0$.

9.3.4 Tensor network method for many-body systems

We have investigated finite-temperature phase transitions in the dodecahedral (20 degrees of freedom) classical Heisenberg model on a two-dimensional square lattice using a large parallelized corner transfer matrix renormalization group (CTMRG) and revealed that the model has a single second-order phase transition with a non-trivial central charge in the conformal field theory between the order and disorder phases. We have also investigated the critical phenomena for intermediate phase associated with Berezinskii-Kosterlitz-Thouless (BKT) phase transitions in the classical six-state clock model on a square lattice using the CTMRG and a finite-m scaling analysis to estimate the Tomonaga-Luttinger parameter. We have confirmed that the intermediate phase is successfully described by the Z_6 dual sine-Gordon model.

In addition, we have optimized a class of tensor network states describable in quantum circuits on one-dimensional quantum spin systems in the thermodynamic limit and found that Suzuki-Trotter-like decomposed unitary operators including optimization parameters coupled with interaction parameters can effectively search the ground state energy rather than employing unitary gates describing an arbitrary unitary transformation. We have developed an MPI parallelized quantum circuit simulator for running these optimizations in a large-scale parallel computing, and succeeded in achieving more than 10 times faster than the existing non-parallelized simulator in a relatively large-scale quantum circuit simulation of 30 qubits.

9.4 Schedule and Future Plan

9.4.1 Large-scale QMC simulations for interacting fermions

The study of topological phenomena has already become a major trend in modern materials science. In order to establish further fundamental concepts and to yet develop new materials, it is important to clarify the correlation effects. In the systems with topological properties, some symmetries play crucial roles to preserve them, and these symmetries often enable us to perform the quantum Monte Carlo calculations without the notorious negative sign problem. We focus on this aspect and launch a new study to elucidate the topological phenomena brought by the strong correlation effect. Specifically, we plan to investigate the properties of high-order topological Mott insulators, which are predicted to exist when the strong correlation is added to the high-order topological insulators, the band insulator with non-trivial topological properties. In conventional topological insulators, when a d-dimensional bulk has a non-trivial topological order, a localized state appears at the edge of the $(d-1)$ dimension, which relation is known as the bulk-edge correspondence. In contrast, in

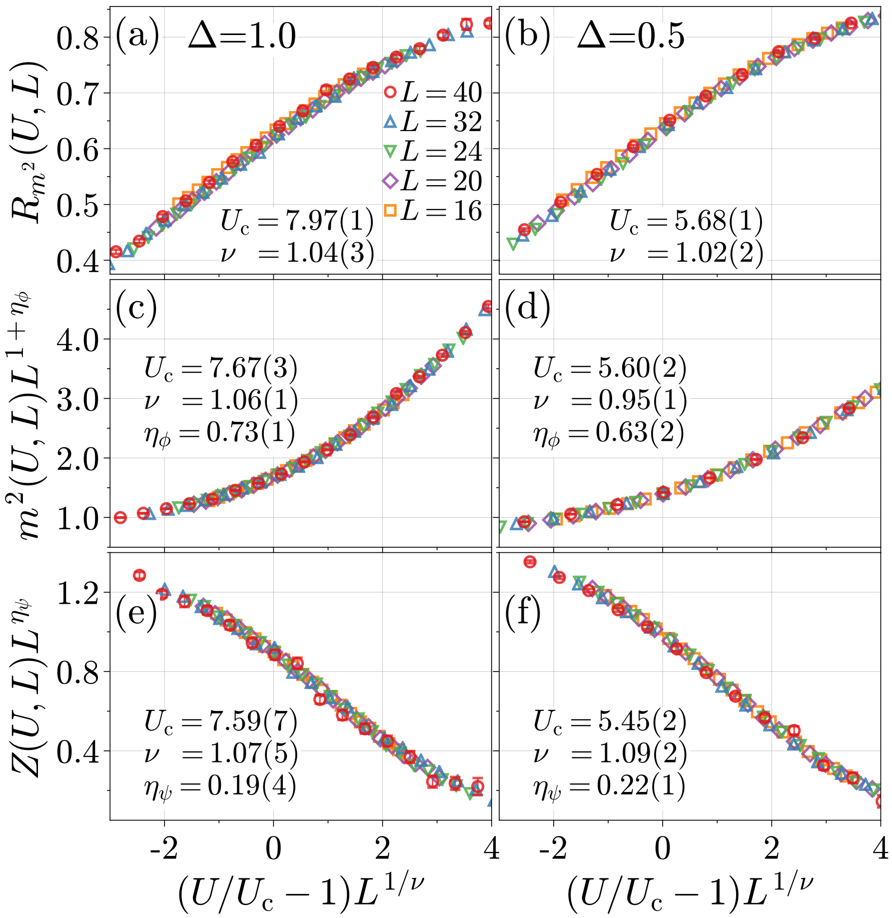

Figure 9.3: Data-collapse fits of correlation ratio [(a) and (b)], staggered magnetization [(c) and (d)], and quasiparticle weight [(e) and (f)]. For each observable, left and right figures show results of $\Delta = 1$ and 0.5 with the same scale. Estimated critical points and exponents are indicated in each figure.

the higher-order topological insulators, localized states with lower dimensionality appear in the $(d-2)$ or $(d-3)$ dimension (e.g., a "corner" state with $d = 0$ if $d = 2$). It has recently been pointed out that although this localized state is band-insulator-like in the non-interacting systems, i.e., there is a gap in both the charge and spin sectors, the strong electron correlation qualitatively changes it to a Mott-like state with a gap opening only in charge [Phys. Rev. Lett 123, 196402 (2019)]. This proposal is based on the result of exact diagonalization for the Kagome lattice, which should be severely limited by finite-size effects and thus was unable to quantitatively estimate the gaps along with the topological phase transition or to determine a precise phase diagram. In this plan, we first aim to clarify the properties of corner states in the Kagome lattice system by the large-scale quantum Monte Carlo simulations. Preliminary calculations have confirmed that the QMC calculations on the Kagome lattice reproduce the results by the exact diagonalization with much fewer computer resources. We also plan to study the pyrochlore system, which is the original setup for the higher-order topological Mott insulators [Nat. Phys. 6, 376 (2009)].

9.4.2 Massively parallel DMRG algorithms for quantum many-body systems

We will optimize our massively parallel DMRG programs to perform calculations effectively and efficiently on Fugaku computer. In addition, we will develop our DMRG programs to perform calculations which are difficult

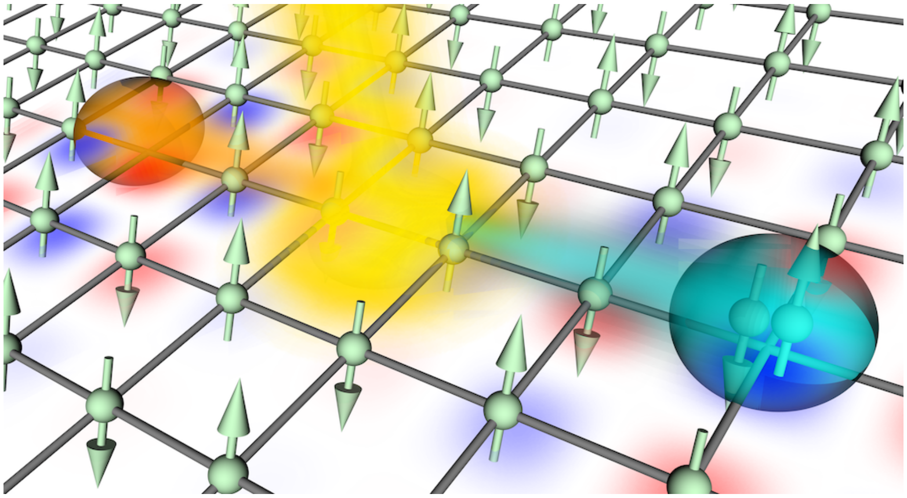

Figure 9.4: A schematic depiction of photoinduced η-pairing.

to perform on K computer, such as finite temperature calculations. Our developed finite temperature DMRG algorithm for higher-dimensional quantum many-body systems requires several ten times larger computational costs compared with those of the ground state calculations. Moreover, we will develop new massively parallel DMRG algorithms, such as the infinite DMRG method for quantum dynamics.

9.4.3 Controlled dynamics in quantum many-body systems

The numerical simulation of quantum dynamics of quantum many-body systems is one of important subjects to bridge the experimental observation and the theoretical prediction. Moreover, as demonstrated in the research results and achievements in this fiscal year, those are also promising fields to find new phenomenona which can be controlled artificially. For example, one of application by using the controlled dynamics includes quantum computation, which has been attracted much attention not only in fundamental scientific fields but also in industrial fields.

In this fiscal year, we have developed a numerical technique to perform the numerically exact simulation in the complex systems composed of the quantum spins and fermion bath system by extending the method originally proposed by two of our members [T. Shirakawa and S. Yunoki, Physical Review B **90**, 195109 (2014)]. We plan to apply this method to study the spin current dynamics in the spin systems coupled to fermions with Rashba spin-orbit coupling, which finds important applications in the field of spintronics.

We also plan to develop quantum-classical hybrid algorithms for quantum computing in order to simulate quantum many-body systems by simulators developed by our team and also by quantum devices.

9.4.4 Tensor network method for many-body systems

We continuously implement the numerical code for calculating physical properties in our parallel CTMRG to clarify the non-trivial criticality in many-body systems and investigate a search algorithm for optimal tensor-network decomposition in non-uniform quantum states, which is important to accelerate the numerical methods based on tensor network algorithm.

We will also investigate quantum (inspired) algorithm with tensor network scheme and quantum circuits in the wake of recent rapid developments in quantum computing (QC). Especially, we focus on HPC-QC hybrid environments and try to accelerate numerical algorithm for simulating static/dynamical property of quantum spin systems.

9.5 Publications

9.5.1 Articles/Journal

[1] B.-H. Kim, K. Seki, T. Shirakawa, and S. Yunoki, "Topological property of a t_{2g}^5 system with a honeycomb lattice structure", Physical Review B **99**, 155135/1–16 (2019).
[2] R. Fujiuchi, T. Kaneko, Y. Ohta, and S. Yunoki, "Photoinduced electron-electron pairing in the extended Falicov-Kimball model", Physical Review B **100**, 045121/1–14 (2019).
[3] S. Ohmura, A. Takahashi, K. Iwano, T. Yamaguchi, K. Shinjo, T. Tohyama, S. Sota, and H. Okamoto, "Effective model of one-dimensional extended Hubbard systems: Application to linear optical spectrum calculations in large systems based on many-body Wannier functions", Physical Review B **100**, 235134/1–15 (2019).
[4] Y. Kawasugi, K. Seki, J. Pu, T. Takenobu, S. Yunoki, H. M. Yamamoto, and R. Kato, "Non-Fermi-liquid behavior and doping asymmetry in an organic Mott insulator interface", Physical Review B **100**, 115141/1–7 (2019).
[5] A. Masaki-Kato, S. Yunoki, and D. S. Hirashima, "Quantum Monte Carlo study of the superfluid density in quasi-one-dimensional systems of hard-core bosons: Effect of the suppression of phase slippage", Physical Review B **100**, 224515/1–7 (2019).
[6] T. Shirakawa, S. Miyakoshi, and S. Yunoki, "Photoinduced η pairing in the Kondo lattice model", Physical Review B **101**, 174307/1–12 (2020).
[7] C. C. Chang, A. Gambhir, T. S. Humble, and S Sota, "Quantum annealing for systems of polynomial equations", Scientific Report **9**, 10258/1–9 (2019).
[8] Y. Kawasugi, K. Seki, S. Tajima, J. Pu, T. Takenobu, S. Yunoki, H. M. Yamamoto, and R. Kato, "Two-dimensional ground-state mapping of a Mott-Hubbard system in a flexible field-effect device", Sci. Adv. **5**, eaav7282 (2019).
[9] H. Watanabe, H. Seo, and S. Yunoki, "Mechanism of superconductivity and electron-hole doping asymmetry in κ-type molecular conductor", Nature Communications **10**, 3167/1–8 (2019).
[10] M. Khazaei, J. Wang, M. Estili, A. Ranjbar, S. Suehara, M. Arai, K. Esfarjani, and S. Yunoki, "Novel MAB phases and insights into their exfoliation into 2D MBenes", Nanoscale. **11**, 11305 (2019).
[11] M. Khazaei, A. Mishra,N. S. Venkataramanan, A. K. Singh, and S. Yunoki, "Recent advances in MXenes: From fundamentals to applications", Curr. Opin. Solid State Mater. Sci. **23**, 164 (2019).
[12] X. Yin, C. S. Tang, S. Zeng, T. C. Asmara, P. Yang, M. A. Naradipa, P. E. Trevisanutto, T. Shirakawa, B. H. Kim, S. Yunoki, M. B. H. Breese, T. Venkatesan, A. T. S. Wee, A. Ariando, and A. Rusydi, "Quantum correlated plasmons and their tunability in undoped and doped Mott-insulator cuprates", ACS Photonics **6**, 3281–3289 (2019).
[13] K. Shinjo, K. Sasaki, S. Hase, S. Sota, S. Ejima, S. Yunoki, and T. Tohyama,"Machine learning phase diagram in the half-filled one-dimensional extended Hubbard model", Journal of Physics Society of Japan **88**, 065001/1–2 (2019).
[14] K. Nishiguchi, T. Shirakawa, H. Watanabe, R. Arita, and S. Yunoki, "Possible Superconductivity Induced by a Large Spin-Orbit Coupling in Carrier Doped Iridium Oxide Insulators: A Weak Coupling Approach", Journal of the Physical Society of Japan **88**, 094701/1–14 (2019).
[15] F. Lange, S. Ejima, T. Shirakawa, S. Yunoki, and H. Fehske, "Block-Lanczos Density-Matrix Renormalization-Group Approach to Spin Transport in Heisenbergt Chains Coupled to Leads", Journal of the Physical Society of Japan **89**, 044601/1–6 (2020).
[16] M. Khazaei, A. Ranjbar, Y. Liang, and S. Yunoki, "Electronic properties and applications of MXenes from ab initio calculations perspective", Chap. 14 in "2D Metal Carbides and Nitrides (MXenes): Structure, Properties and Applications", ed. by B. Anasori and Y. Gogotsi (Springer, 2019).
[17] T. Kaneko, T. Shirakawa, and S. Yunoki, "Photo-induced η-pairing states in the Hubbard model", Kotai Butsuri **55**, 1–9 (2020) (in Japanese).

9.5.2 Invited Talks

[1] S. Sota,"Development of massively parallel DMRG method and its applications to quantum dynamics", ISSP supercomputer center and CCMS collaboration workshop "Novel development of condensed matter physics", April 2–3 (2019), Kashiwa (Japan).
[2] S. Yunoki, "Correlation-driven dimerization and topological gap opening in isotropically strained graphene", International Workshop: Topology the New Horizon of Materials Science and Nanophotonics, June 12-13 (2019), NIMS, Tsukuba (Japan).

[3] S. Yunoki, "Photoinduced superconductivity by η-pairing mechanism in a Mott insulator", 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10), July 22-26 (2019), City University of Hong Kong, Hong Kong (China).
[4] H. Ueda, "Analysis of critical phenomena in classical spin systems using large-scale parallelized corner transfer matrix renormalization group", the 4th HPC-Phys workshop, August 26 (2019), Kobe (Japan).
[5] S. Yunoki, "Photoinduced superconductivity by η pairs in a Mott insulator", International Conference Electron Correlation in Superconductors and Nanostructures (ECSN-2019), October 6-10 (2019), Odessa (Ukraine).
[6] Y. Otsuka, "QMC study of the Gross-Neveu universality class; the chiral-Heisenberg class revisited", Mini-workshop on "Fermion Quantum Criticality and beyond", February 13–14 (2020), Würzburg (Germany).
[7] S. Yunoki, "Relativistic Mott insulator, superconductivity, and other exotic states in $5d$ electrons", Mini-workshop on "Fermion Quantum Criticality and beyond", February 13–14 (2020), Würzburg (Germany).

9.5.3 Oral Talks

[1] H. Ueda, "Critical behavior of the two-dimensional dodecahedron model", CAQMP 2019 (Computational Approaches to Quantum Many-body Problems), July 29 (2019), Kashiwa (Japan).
[2] Y. Otsuka, K. Seki, S. Yunoki, and S. Sorella, "Numerical study of universal quantum criticality in strongly correlated Dirac electrons", IMS workshop on "Topological physics and organic massless Dirac systems", August 8–9 (2019), Okazaki (Japan).
[3] Y. Otsuka, K. Seki, S. Yunoki, and S. Sorella, "Numerical study of Mott transition in the Hubbard model with d-wave superconducting order parameter", Autumn Meeting of Physics Society of Japan, September 10-13 (2019), Gifu (Japan).
[4] T. Tohyama, S. Sota, S. Yunoki,"Dynamical DMRG Study of spin dynamics on $t-t'-J$ model", Autumn Meeting of Physics Society of Japan, September 10–13 (2019), Nagoya (Japan).
[5] T. Yamaguchi, K. Iwano, S. Ohmura, A. Takahashi, K. Shinjo, T. Tohyama, S. Sota, H. Okamoto, "Theoretical prediction for an optical conductivity of a charge model in the thermodynamic limit by constructing the many-body Wannier functions", Autumn Meeting of Physics Society of Japan, September 10–13 (2019), Nagoya (Japan).
[6] S. Ohmura, A. Takahashi, T. Yamaguchi, K. Iwano, K. Shinjo, T. Tohyama, S. Sota, H. Okamoto, "Charge model: An effective model for the one-dimensional extended Hubbard model, where spin-charge separation is compatible with charge fluctuations", September 10–13 (2019), Nagoya (Japan).
[7] K. Shinjo, S. Sota, T. Tohyama, "Time-dependent DMRG study of optical conductivity on one-dimensional and ladder lattice extended Hubbad model", September 10–13 (2019), Nagoya (Japan).
[8] H. Ueda, K. Okunishi, S. Yunoki, T. Nishino, "Finite-m scaling of corner transfer matrix renormalization group for entanglement spectrum", 2019 Autumn Meeting, The Physical Society of Japan, September 10-13 (2019), Nagoya (Japan).
[9] H. Ueda, "Roles of easy-plane and easy-axis XXZ anisotropy and bond alternation in a frustrated ferromagnetic spin-1/2 chain", the 14th quantum-spin-system workshop, January 8 (2020), Semboku (Japan).
[10] T. Shirakawa, "Simulations of dynamics in quantum many-body systems", The 190th R-CCS Cafe, February 3 (2020), Kobe (Japan).
[11] S. Sota, T. Shirakawa, S. Yunoki, T. Tohyama, "Dynamical DMRG study of spin excitation dynamics in triangular lattice spin-1/2 antiferromagnet", APS March Meeting 2020, March 2–6 (2020), Denver (USA).
[12] T. Shirakawa, S. Miyakoshi, and S. Yunoki, "Photo-induced superconductivity in the Kondo lattice", APS March Meeting 2020, March 2–6 (2020), Denver (USA).
[13] H. Ueda, Y. Otsuka, M. Nakata, "Variational method using matrix product unitary state", 75th Annual Meeting, The Physical Society of Japan, March 16-19 (2020), Nagoya (Japan).

9.5.4 Posters

[1] S. Sota, S. Yunoki, "Kernel polynomial expansion method on quantum computer", Autumn Meeting of Physics Society of Japan, September 10–13 (2019), Nagoya (Japan).
[2] T. Shirakawa, S. Sota, S. Yunoki, and T. Tohyama, "Dynamical spin structure factor of the triangular-lattice Heisenberg model", 2019 Autumn Meeting of the Physical Society of Japan, September 10–13 (2019), Gifu (Japan).
[3] H. Watanabe, T. Shirakawa, K. Seki, H. Sakakibara, and S. Yunoki, "Study for magnetism and superconductivity in high-T_c cuprates using 4-band d-p model", 2019 Autumn Meeting of the Physical Society of Japan, September 10–13 (2019), Gifu (Japan).

[4] K. Seki, T. Shirakawa, and S. Yunoki, "Variational cluster approach to thermodynamic properties of interacting fermions at finite temperatures", 2019 Autumn Meeting of the Physical Society of Japan, September 10–13 (2019), Gifu (Japan).
[5] S. Sota, T. Shirakawa, S. Yunoki, T. Tohyama, "Dynamical DMRG Study of Spin Excitation Dynamics on the Triangular Lattice Antiferromagnetic Heisenberg model", International Conference on Strongly Correlated Electron Systems 2019, September 23–28 (2019), Okayama (Japan).

9.5.5 Software

[1] S. Sota, K. Morita, H. Matsueda, S. Yunoki, T. Tohyama, "DDMRG (Dynamical DMRG)", R-CCS software.
[2] S. Sota, S. Yunoki, T. Tohyama, "2-D DMRG", R-CCS software.
[3] S. Sota, Y. Imamura, T. Nakajima, S. Yunoki, T. Tohyama, "paraDMRG", R-CCS software.
[4] S. Sota, S. Yunoki, "QUARTZ", R-CCS software.