Field Theory Research Team

1. Team members

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2. Research Activities

Our research field is physics of elementary particles and nuclei, which tries to answer questions in history of mankind: What is the smallest component of matter and what is the most fundamental interactions? This research subject is related to the early universe and the nucleosynthesis through Big Bang cosmology. Another important aspect is quantum properties, which play an essential role in the world of elementary particles and nuclei as well as in the material physics at the atomic or molecular level. We investigate nonperturbative properties of elementary particles and nuclei through numerical simulations with the use of lattice QCD (Quantum ChromoDynamics). The research is performed in collaboration with applied mathematicians, who are experts in developing and improving algorithms, and computer scientists responsible for research and development of software and hardware systems.

Lattice QCD is one of the most advanced case in quantum sciences: Interactions between quarks, which are elementary particles known to date, are described by QCD formulated with the quantum field theory. We currently focus on two research subjects: (1) QCD at finite temperature and finite density. We try to understand the early universe and the inside of neutron star by investigating the phase structure and the equation of state. (2) First principle calculation of nuclei based on QCD. Nuclei are bound states of protons and neutrons which consist of three quarks. We investigate the hierarchical structure of nuclei through the direct construction of nuclei in terms of quarks.

Successful numerical simulations heavily depend on an increase of computer performance by improving algorithms and computational techniques. However, we now face a tough problem that the trend of computer architecture becomes large-scale hierarchical parallel structures consisting of tens of thousands of nodes which individually have increasing number of cores in CPU and arithmetic accelerators with even higher degree of parallelism: We need to develop a new type of algorithms and computational techniques, which should be different from the conventional ones, to achieve better computer performance. For optimized use of K computer our research team aims at (1) developing a Monte Carlo algorithm to simulate physical system with negative weight effectively and (2) improving iterative methods to solve large system of linear equations. These technical development and improvement are carried out in the research of physics of elementary particles and nuclei based on lattice QCD.

3. Research Results and Achievements

3.1. QCD at finite temperature and finite density

Establishing the QCD phase diagram spanned by the temperature T and the quark chemical potential μ in a quantitative way is an important task of lattice QCD. We are currently working on tracing the critical line in the parameter space of temperature, chemical potential and quark mass in 3 flavor QCD using the O(a) improved Wilson quark action and the Iwasaki gauge action. As a first step we have determined the critical end point at zero chemical potential $\mu=0$. Our strategy is to identify at which temperature the Kurtosis of physical observable measured at the transition point on several different spatial volumes intersects. This method is based on the property of opposite spatial volume dependences of the Kurtosis at the transition point between the first order phase transition side and the crossover one. We have obtained T_E=133(2)(1)(3) MeV and $m_{PS,E}$=306(7)(14)(7) MeV for the temperature and the pseudoscalar meson mass at the critical end point. This is the world's first determination of the critical end point in 3 flavor QCD and a significant step forward in our understanding of the phase diagram. As a next step we have investigated the phase structure in the presence of finite chemical potential $\mu\neq 0$. We first focus on extracting the curvature of the critical line on the μ/T-$(m_{PS})^2$ plane. The strategy to determine the critical end point at fixed finite μ is the same as the $\mu=0$ case. Note that we incorporate the phase contribution coming from the quark determinant with $\mu\neq 0$ by the reweighting method. We evaluate the phase of the determinant exactly by developing an efficient numerical method with the use of a dimensional reduction technique in the temporal direction. We also employ the multi-parameter reweighting method to trace the critical line in a wide range of the chemical potential. Figure 1 shows the behavior of the critical line in the μ/T-$(m_{PS})^2$ plane. Red and blue symbols denote two choices of the physical input to determine the lattice cutoff so that their difference represents a systematic uncertainty in the scale determination. We clearly observe the curvature of the critical line. Its value is extracted from the following fit form:

$$\left(\frac{m_{\mathrm{PS,E}}(\mu)}{m_{\mathrm{PS,E}}(0)}\right)^2 = 1+\alpha_1\left(\frac{\mu}{\pi T_{\mathrm{E}}(0)}\right)^2+\alpha_2\left(\frac{\mu}{\pi T_{\mathrm{E}}(0)}\right)^4$$

We obtain α_1=1.924(60) and α_1=2.148(39) for red and blue symbols, respectively.

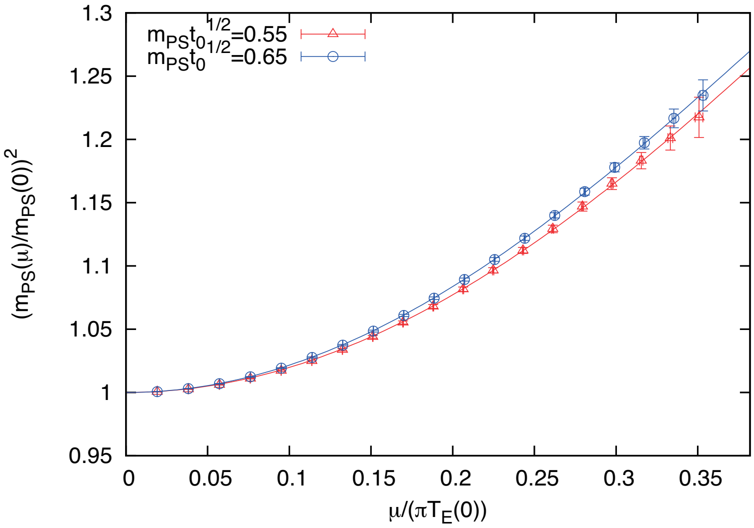

Figure 1: Critical line in the μ /T-$(m_{PS})^2$ plane. Red and blue symbols denote two choices of the scale setting.

3.2. Nuclei in lattice QCD

In 2010 we succeeded in a direct construction of the ^{4}He and ^{3}He nuclei from quarks and gluons in lattice QCD for the first time in the world. Calculations were carried out at a rather heavy degenerate up and down quark mass corresponding to m_π=0.8 GeV in quenched QCD to control statistical errors in the Monte Carlo evaluation of the helium Green's functions. As a next step we investigated the dynamical quark effects on the binding energies of the helium nuclei, the deuteron and the dineutron. We performed a 2+1 flavor lattice QCD simulation with the degenerate up and down quark mass corresponding to m_π=0.51 GeV. To distinguish a bound state from an attractive scattering state, we investigate the spatial volume dependence of the energy difference between the ground state and the free multi-nucleon state by changing the spatial extent of the lattice from 2.9 fm to 5.8 fm. We observed that the measured ground states for all the channels are bound. This result raises an issue concerning the quark mass dependence. At the physical quark mass, namely in experiment, there is no bound state in the dineutron channel. So we expect that the bound state in the dineutron channel observed in our simulation at m_π=0.51 GeV may disappear at some quark mass toward the physical value. We have investigated the quark mass dependence performing a simulation at m_π=0.30 GeV. Figure 2 show the $(m_\pi)^2$ dependence of the binding energies for ^{4}He nucleus (top left), ^{3}He nucleus (top right), deuteron (bottom left) and dineutron (bottom right) channels. Green star in each panel denotes the experimental value. We find that the ground states in all channels are bound states. Their binding energies show rather weak quark mass dependence in the region from m_π=0.30 GeV to 0.51 GeV. The difference we observe from experiment may arise from various sources, either physical or computational in origin. A possible physical one is the heavier quark mass than experiment. Our results yield smaller binding energy in the dineutron channel than the deuteron channel in both cases of m_π=0.30 GeV to 0.51 GeV so that the former bound state may become unbound for further decrease of m_π. On the computational side, finite lattice spacing effects could be rather subtle. The repulsive property between the nucleons in the short distance, which is known to be important for the nucleus structure, could be strongly affected by such effects.

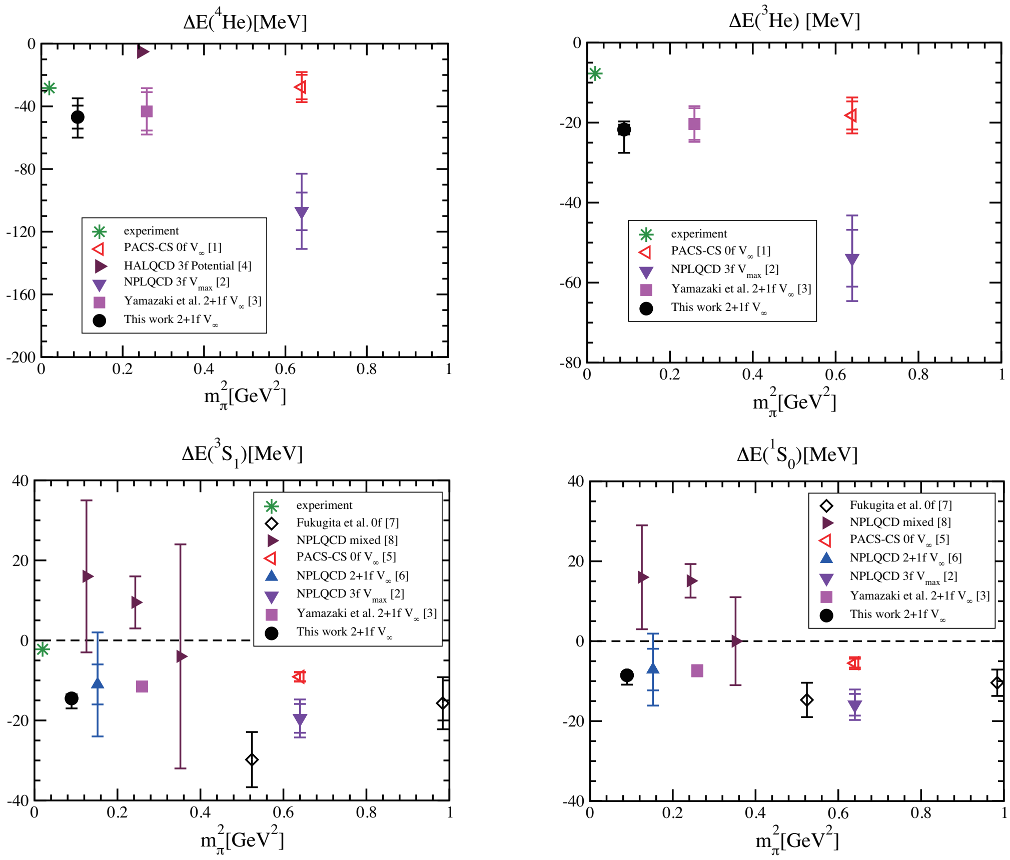

Figure 2: Binding energies for ^{4}He nucleus (top left), ^{3}He nucleus (top right), deuteron (bottom left) and dineutron (bottom right) channels as a function of $(m_\pi)^2$. Green star denotes the experimental value in each channel.

3.3. Development of algorithms and computational techniques

3.3.1. Application of z-Pares to lattice QCD on K computer

Eigenvalue problem for given large sparse matrix is common across various computational sciences including lattice QCD. Sakurai group in University of Tsukuba, who has been working on the eigenvalue problem for sparse matrices for a long time, is now developing a software package for massively parallel eigenvalue computation for sparse matrices called z-Pares (short for Complex

Moment-based Parallel Eigen-Solvers). From this fiscal year we started to apply z-Pares to a large scale calculation of lattice QCD on K computer. We have to solve the Wilson-Dirac equation Ax=b in lattice QCD, where A is an N×N complex sparse non-Hermitian matrix with N the number of four dimensional space-time sites multiplied by 12. In current typical simulations the dimension N is $O(10^9)$. z-Pares implements a complex moment based contour integral eigensolver. It computes eigenvalues inside a user-specified contour path on the complex plane and corresponding eigenvectors. In most cases of lattice QCD calculations our interest is restricted to O(10) eigenvalues around the origin so that lattice QCD should be a good example of application of z-Pares. Figure 3 shows a test result using a $12^3\times24$ lattice. Red circles denote the discretized contour consisting of 32 points on a circle with the radius of 0.01. We can obtain the eigenvalues and corresponding eigenvectors inside the contour. In Fig. 3 we find 8 eigenvalues denoted by black plus symbol. At present we work on tuning of algorithmic parameters in z-Pares using small or medium sizes of lattices. In next fiscal year, we plan to apply z-Pares to a 96^4 lattice used for a state-of-the-art calculation in lattice QCD.

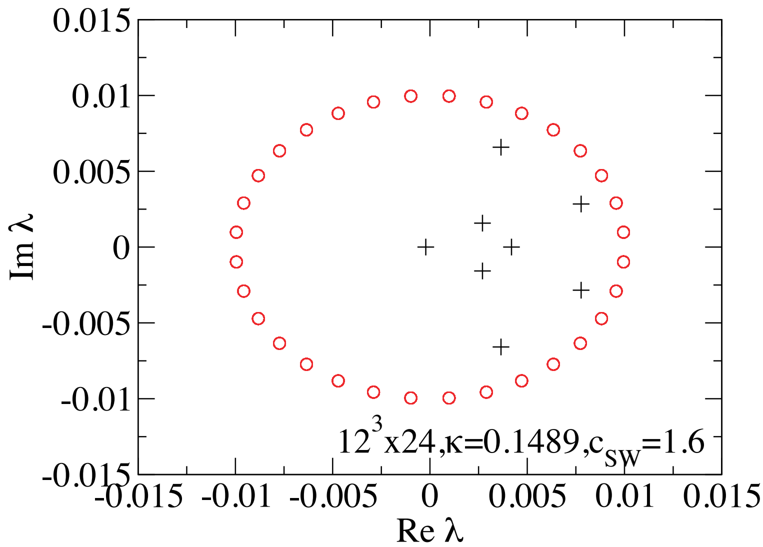

Figure 3: Eigenvalues of a Wilson-Dirac matrix with the lattice size of $12^3\times24$ around the origin in the complex plane. κ and c_{SW} denote the parameters to control the properties of the Wilson-Dirac matrix. Red circles denote the discretized contour on a circle with the radius of 0.01. Black plus symbol denotes the eigenvalues obtained by z-Pares.

3.3.2. Algorithm to simulate physical system with negative weight in path-integral formalism

The Monte Carlo simulation of lattice gauge theory is quite powerful to study nonperturbative phenomena of particle physics. However, when the action has an imaginary part like the θ term, it suffers from the numerical sign problem, failure of usual importance sampling techniques. The effect of the θ term on non-Abelian gauge theory, especially quantum chromodynamics (QCD) is important, because it is related to a famous unsolved problem, “strong CP problem”. The difficulty is also shared with finite density lattice QCD. So development of effective techniques to solve or by-pass the sign problem leads to a lot of progress in the study of the QCD phase diagram at finite temperature and density. It is well-known that the θ term has a non-trivial contribution to Abelian gauge theory in two dimensions, too. Coleman argued that the (massive) Schwinger model, 2D QED, undergoes a phase transition at $\theta = \pi$ as m=g increases where m is the fermion mass and g is the coupling constant. Figure 4 illustrates the expected phase diagram of the Schwinger model with the θ term. Recently we successfully applied the Grassmann tensor renormalization group (GTRG) to the analysis on the one-flavor lattice Schwinger model in the Euclidean formulation. The GTRG method directly treats the Grassmann numbers without relying on the pseudofermion technique employed in the conventional hybrid Monte Carlo algorithm so that the computational cost is comparable to the bosonic case. Another virtue is that it does not suffer from the sign problem caused by the fermion determinant. We have extended the GTRG method to the case including the θ term, where the action becomes complex, and have succeeded in reproducing the expected phase structure at $\theta = \pi$ depicted in Fig. 4: When the fermion mass is large, there exists a first order phase transition and it terminates at m_c which has a second order phase transition belonging to the Ising universality class. It is shown that the GTRG is applicable to the physical system whose action is a complex number.

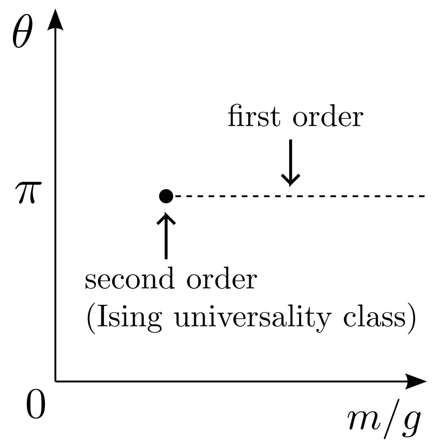

Figure 4: Expected phase diagram of Schwinger model with the θ term. The dotted line denotes a first order phase transition, which terminates at a second order phase transition point belonging to the Ising universality class.

4. Schedule and Future Plan

4.1. QCD at finite temperature and finite density

We are now investigating the critical surface in the parameter space of temperature, chemical potential and quark masses in 3flavor QCD. After that, we plan to explore the study of the phase structure in 2+1 flavor QCD with the finite size scaling analysis.

4.2. Nuclei in lattice QCD

Our results at m_π=0.30 GeV in 2+1 flavor QCD show that the dineutron channel seems still bound. We currently make a large scale simulation at or around the physical quark mass. We also plan to investigate the possible systematic errors due to the finite lattice spacing.

4.3. Development of algorithms and computational techniques

4.3.1. Application of z-Pares to lattice QCD on K computer

In collaboration with Sakurai group at University of Tsukuba we plan to apply z-Pares to a 96^4 lattice used for a state-of-the-art calculation in lattice QCD.

4.3.2. Algorithm to simulate physical system with negative weight in path-integral formalism

We have demonstrated that the GTRG method is efficient even for the complex action employing the Schwinger model with the θ term. Next step is an extension to various spin models and non-Abelian lattice gauge theories on higher dimensions.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. X.-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, "Critical endpoint of the finite temperature phase transition for three flavor QCD", Physical Review D91 (2015) 014508.
2. X.-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, " Curvature of the critical line on the plane of quark chemical potential and pseudo scalar meson mass for three-flavor QCD", arXiv:1503.00113 [hep-lat].
3. R. Horsley, Y. Nakamura, A. Nobile, P.E.L. Rakow, G. Schierholz, and J.M. Zanotti, "Nucleon axial charge and pion decay constant from two-flavor lattice QCD", Physics Letters B732 (2014) 41.
4. P.E. Shanahan, A.W. Thomas, R.D. Young, J.M. Zanotti, R. Horsley, Y. Nakamura, D. Pleiter, P.E.L. Rakow, G. Schierholz, and H. Stüben, "Magnetic form factors of the octet baryons from lattice QCD and chiral extrapolation", Physical Review D89 (2014) 074511.
5. A. J. Chambers, R. Horsley, Y. Nakamura, H. Perlt, D. Pleiter, P. E. L. Rakow, G. Schierholz, A. Schiller, H. Stüben, R. D. Young, and J. M. Zanotti, "Feynman-Hellmann approach to the spin structure of hadrons", Physical Review D90 (2014) 014510.
6. A.J. Chambers, R. Horsley, Y. Nakamura, H. Perlt, P.E.L. Rakow, G. Schierholz, A. Schiller, and J.M. Zanotti, "A novel approach to nonperturbative renormalization of singlet and nonsinglet lattice operators", Physics Letters B740 (2014) 30.

7. P. E. Shanahan, R. Horsley, Y. Nakamura, D. Pleiter, P. E. L. Rakow, G. Schierholz, H. Stüben, A. W. Thomas, R. D. Young, and J. M. Zanotti (CSSM and QCDSF/UKQCD Collaborations), "Determination of the strange nucleon form factors", Physical Review Letters 114 (2015) 091802.
8. Yuya Shimizu and Yoshinobu Kuramashi, "Critical behavior of the lattice Schwinger model with a topological term at $\theta = \pi$ using the Grassmann tensor renormalization group", Physical Review D90 (2014) 014508.
9. Yuya Shimizu and Yoshinobu Kuramashi, "Grassmann tensor renormalization group approach to one-flavor lattice Schwinger model", Physical Review D90 (2014) 074503.
10. H. Suno, Y. Suzuki, and P. Descouvemont, "Triple-α continuum structure and Hoyle resonance of ^{12}C using the hyperspherical slow variable discretization", Physical Review C91 (2015) 014004.
11. H. Suno and B. D. Esry, "Cold elastic and reactive atom-molecule collisions in helium−helium−alkali-metal triatomic systems", Physical Review A89 (2014) 052701.
12. Takeshi Yamazaki, Ken-ichi Ishikawa, Yoshinobu Kuramashi, and Akira Ukawa "Study of quark mass dependence of binding energy for light nuclei in 2+1 flavor lattice QCD", arXiv:1502.04182 [hep-lat].
13. Shinji Takeda and Yusuke Yoshimura, "Grassmann tensor renormalization group for one-flavor lattice Gross-Neveu model with finite chemical potential", Progress of Theoretical and Experimental Physics (2015) 043B01.

(2) Conference Papers

1. Y. Nakamura, X.-Y. Jin, Y. Kuramashi, S. Takeda, and A. Ukawa, "Update on the critical endpoint of the finite temperature phase transition for three flavor QCD with clover type fermions", Proceedings of Science (LATTICE2014) 194.
2. R. Horsley, J. Najjar, Y. Nakamura, H. Perlt, D. Pleiter, P.E.L. Rakow, G. Schierholz, A. Schiller, H. Stüben, and J.M. Zanotti, "Determining Sigma - Lambda mixing", Proceedings of Science (LATTICE2014) 110.
3. A. Chambers, R. Horsley, Y. Nakamura, H. Perlt, D. Pleiter, P.E.L. Rakow, G. Schierholz, A. Schiller, H. Stuben and R.D. Young, and J. Zanotti, "Connected and disconnected quark contributions to hadron spin", Proceedings of Science (LATTICE2014) 165.
4. X.-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, "Scalar correlators near the 3-flavor thermal critical point", Proceedings of Science (LATTICE2014) 195.
5. Takeshi Yamazaki, "Hadronic Interactions", Proceedings of Science (LATTICE2014) 009.
6. S. Takeda, X-Y. Jin, Y. Kuramashi, Y. Nakamura, and A. Ukawa, "Critical end point in Nf=3 QCD with finite density and temperature", Proceedings of Science (LATTICE2014)

196.

(3) Invited Talks

1. Y. Kuramashi, "Lattice QCD", US/Japan Exascale Applications Workshop, Gatlinburg, Tennessee, USA, Sep. 5-6, 2015.
2. Y. Kuramashi, "2+1 Flavor Lattice QCD Simulation on K Computer" CCS-BNL Workshop on Lattice Gauge Theories 2015 (CCS-BNL LGT 2015), University of Tsukuba, Tsukuba, Japan, March 12-13, 2015.
3. Y. Nakamura, "Critical endpoint of finite temperature phase transition for three flavor QCD" CCS-BNL Workshop on Lattice Gauge Theories 2015 (CCS-BNL LGT 2015), University of Tsukuba, Tsukuba, Japan, March 12-13, 2015.
4. Yuya Shimizu, "Tensor Renormalization Group Study of Lattice Schwinger Model", Seminar at Kyushu University, Apr. 11, 2014.
5. Yuya Shimizu, "Tensor Renormalization Group Study of Lattice Schwinger Model", Seminar at Nagoya University, Jul. 8, 2014.
6. Yuya Shimizu, "Tensor Renormalization Group Study of Lattice Schwinger Model", Seminar at Osaka University, Jul. 15, 2014.
7. Yuya Shimizu, "Introduction to Grassmann Tensor Renormalization Group in Low-Dimensional Lattice Gauge Theory", Seminar at Okayama Institute for Quantum Physics, Aug. 6, 2014.
8. Yuya Shimizu, "Tensor Renormalization Group Approach to Lattice Gauge Theory", Seminar at University of Tsukuba, Nov. 7, 2014.
9. Takeshi Yamazaki, "Hadronic Interactions", 32nd International Symposium on Lattice Field Theory, Columbia University, New York, June 23-28 2014.
10. Takeshi Yamazaki, "Hadronic interaction and beyond standard model from lattice gauge theory", Progress in Particle Physics 2014, Kyoto University, Kyoto, July 28-August 1 2014.
11. Takeshi Yamazaki, "Light nuclei from lattice QCD", Advances and perspectives in computational nuclear physics, Hilton Waikoloa Village, Hawaii, October 5-7 2014.
12. Takeshi Yamazaki, "格子 QCD を用いた原子核直接計算", RCNP workshop on QCD を基礎とする核子多体系物理の理解, Osaka University, Osaka, December 19-20 2014.
13. Takeshi Yamazaki, "Light nuclei from lattice QCD", RIKEN BNL Research Center workshop on Multi-Hadron and Nonlocal Matrix Elements in Lattice QCD, Brookhaven National Laboratory, NY, February 5-6 2015.
14. Takeshi Yamazaki, "格子 QCD を用いた軽い原子核の計算", 素粒子・原子核・宇宙「京からポスト京に向けて」シンポジウム, Kioi forum, Tokyo, March 11-12 2015.

15. Shinji Takeda, "Curvature of critical line in m_π-μ plane for 3-flavor QCD", CCS-BNL Workshop on Lattice Gauge Theories 2015 (CCS-BNL LGT 2015), University of Tsukuba, Tsukuba, Japan, March 12-13, 2015.

(4) Posters and presentations

1. Y. Nakamura, "Update on the critical endpoint of the finite temperature phase transition for three flavor QCD with clover type fermion" (talk), 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, Jun. 23-28, 2014.
2. Y. Nakamura, "The critical end-point of the finite temperature phase transition in three flavor QCD" (talk), XQCD14, June 19–21, 2014, Stony Brook University, New York, USA.
3. H. Suno, Y. Suzuki, and P. Descouvemont, "Triple-α continuum structure and Hoyle resonance of 12C using the hyperspherical slow variable discretization" (talk), 2015 Annual Meeting of the Physical Society of Japan, Waseda University, Tokyo, Japan, March 21-24, 2015.
4. H. Suno, Y. Nakamura, K.-I. Ishikawa, and Y. Kuramashi, "Block BiCGSTAB for lattice QCD on the K computer" (poster), The 5th AICS International Symposium, RIKEN AICS, Kobe, Japan, December 8-9, 2014.
5. H. Suno, N. Sakumichi E. Hiyama, "Theoretical study of helium triatomic systems using hyperspherical coordinates" (talk), 2014 Autumn Meeting of the Physical Society of Japan, Chubu University, Kasugai, Japan, September 7-10, 2014.
6. X.-Y. Jin, "Scalar correlators near the 3-flavor thermal critical point" (talk), 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, Jun. 23-28, 2014.
7. Yuya Shimizu, "Grassmann Tensor Renormalization Group Study of Lattice QED with θ Term in Two Dimensions" (talk), 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, Jun. 23-28, 2014.
8. Yuya Shimizu, "Numerical Analysis of Lattice Schwinger Model Including θ Term Using Tensor Renormalization Group" (poster), Progress in Particle Physics 2014, Kyoto University, Kyoto, Jul. 28-Aug. 1, 2014.
9. Yuya Shimizu, "Numerical Analysis of Phase Structure of Two-Dimensional Lattice QED in θ Vacuum" (talk), 2014 Autumn Meeting of the Physical Society of Japan, Saga University, Sep. 18-21, 2014.
10. Shinji Takeda, " Critical end point in Nf=3 QCD with finite density and temperature" (talk), 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, Jun. 23-28, 2014.

11. Takeshi Yamazaki, "Light nuclei from 2+1 flavor lattice QCD" (talk), Hadrons and Hadron Interactions in QCD 2015, Kyoto University, Kyoto, February 15-March 21 2015.

(5) Patents and Deliverables

1. H. Suno, Y. Nakamura, K.-I. Ishikawa, and Y. Kuramashi, "Block BiCGStab for lattice QCD on the K computer", AICS Technical Report No. 2014-001.
2. H. Suno, Y. Nakamura, Y. Kuramashi, Y. Futamura, and T. Sakurai, "Optimization of matrix-vector multiplication for Real-Space Density Functional Theory Code on the K computer", AICS Technical Report No. 2014-002.
3. S. Takeda, Y. Kuramashi, and Y. Nakamura, "An efficient algorithm for the computation of the reduced determinant for Wilson-Dirac operator", AICS Technical Report No. 2015-001.