Chapter 5

Field Theory Research Team

5.1 Members

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5.2 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.

5.3 Research Results and Achievements

5.3.1 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 have been working on tracing the critical end line in the parameter space of temperature, chemical potential and quark masses in 3 and 2+1 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 $\mu = 0$ in 3 flavor case. 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 $T_{\rm E}$=133(2)(1)(3) MeV and $m_{\rm PS,E}$=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 providing 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 $\mu \neq 0$ in 3 flavor QCD[4]. We have successfully determined the curvature of the critical end line on the μ/T-$(m_{\rm PS})^2$ plane near the vanishing chemical potential employing the Kurtosis intersection method and the multi-parameter reweighting method. After the investigation with and without the chemical potential in 3 flavor QCD, we embark on the determination of the critical end line of the finite temperature phase transition in 2+1 flavor QCD. We first focus on the behavior of the critical end line around the SU(3) symmetric point ($m_{\rm ud} = m_{\rm s}$) at the temporal size $N_T = 6$ with the lattice spacing as low as $a \approx 0.19$ fm[5]. Figure 5.1 plots the critical end line on the m_π^2-$m_{\eta_s}^2$ plane, where the pink line indicates $m_{\rm ud} = m_{\rm s}$ ($m_\pi = m_{\eta_s}$). We confirm that the slope of the critical end line takes the value of -2 at the SU(3) symmetric point, and find that the second derivative is positive. At present our investigation is extended to wider range of quark masses away from the SU(3) symmetric point.

5.3.2 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 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. A new simulation at m_π=0.30 GeV, however, reveals that the ground states in all channels are bound states showing rather weak quark mass dependence in the region from m_π=0.30 GeV to 0.51 GeV[9]. In order to understand the quark mass dependence more systematically, we are currently working on the calculation of the binding energies for the helium nuclei, the deuteron and the dineutron at the physical point on a 96^4 lattice. Figure 5.2 shows a preliminary result for the effective energy difference of ^{3}He nuclei, which should represent the binding

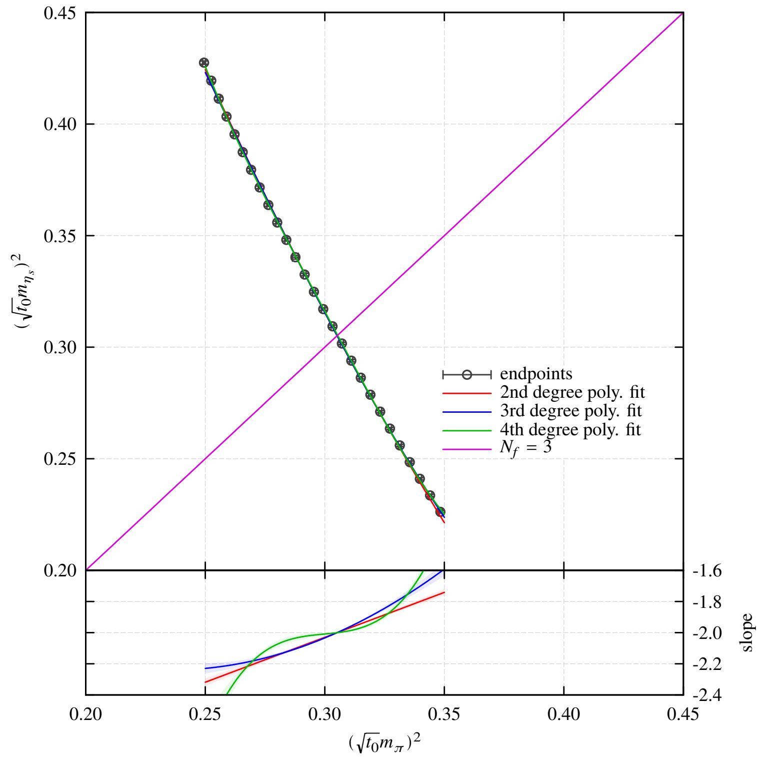

Figure 5.1: Critical end line on the m_π^2-$m_{\eta_s}^2$ plane (top) and the slope along the critical end line (bottom). $\sqrt{t_0}$ denotes the Wilson flow scale.

energy in large time region. Although the statistical precision is not sufficient at this stage, we plan to diminish the error bars with increasing statistics.

5.3.3 Development of algorithms and computational techniques

Application of z-Pares to lattice QCD on K computer

Eigenvalue problem for a 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). We have applied z-Pares to a large scale calculation of lattice QCD on K computer. We need to solve the Wilson-Dirac equation $D\vec{x} = \vec{b}$ in lattice QCD, where D is an $N \times N$ 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 discretized 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 5.3 shows a test study comparing the analytic results (black crosses) and the numerical ones (red circles) for the eigenvalues of the free (without interactions with gauge fields) Wilson-Dirac matrix on a 96^4 lattice. We observe both results show good agreement inside the contour. In Fig. 5.4 we plot the numerical results for the eigenvalues of the $O(a)$-improved Wilson-Dirac matrix on a 96^4 lattice used for a state-of-the-art calculation in lattice QCD, whose configuration properties are explained in Ref. [15]. We find four eigenvalues (red circles) near the origin. We are now working on an algorithmic improvement to efficiently solve the shifted Wilson-Dirac equation on the discretized contour.

Tensor network scheme 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 component like the θ

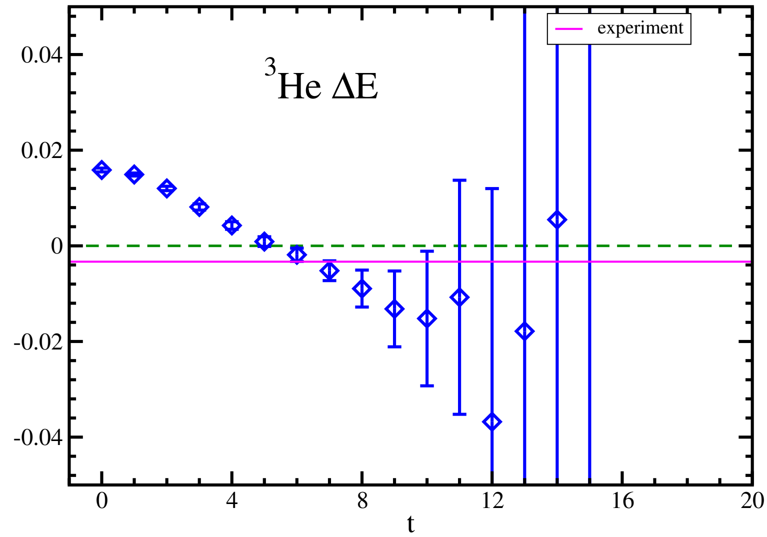

Figure 5.2: Effective energy difference for ^{3}He nuclei as a function of time. Solid line indicates the experimental result for the binding energy.

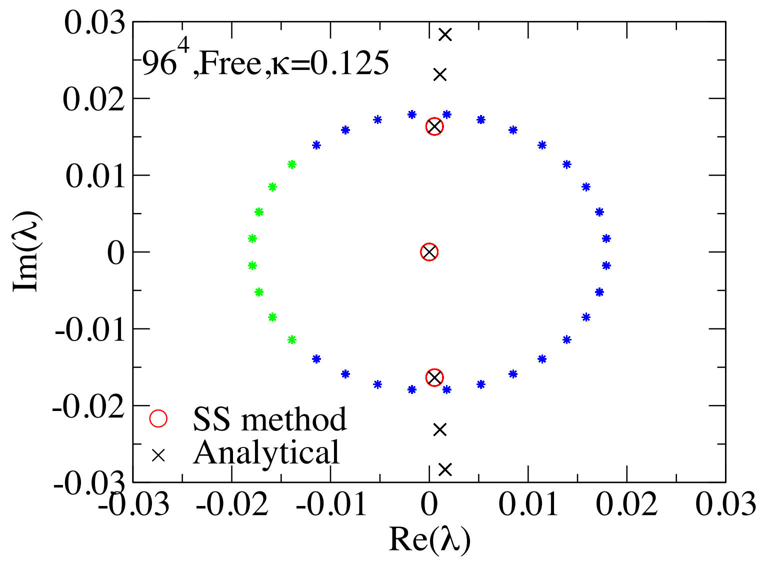

Figure 5.3: Eigenvalue distribution of the free (without interactions with gauge fields) Wilson-Dirac matrix on a 96^4 lattice. κ is a parameter to control the mass of the Wilson quark. Green and Blue star symbols denote the discretized contour around the origin of the complex plane. Black crosses denote the analytic results for the eigenvalues and red circles is for the numerical ones obtained by z-Pares.

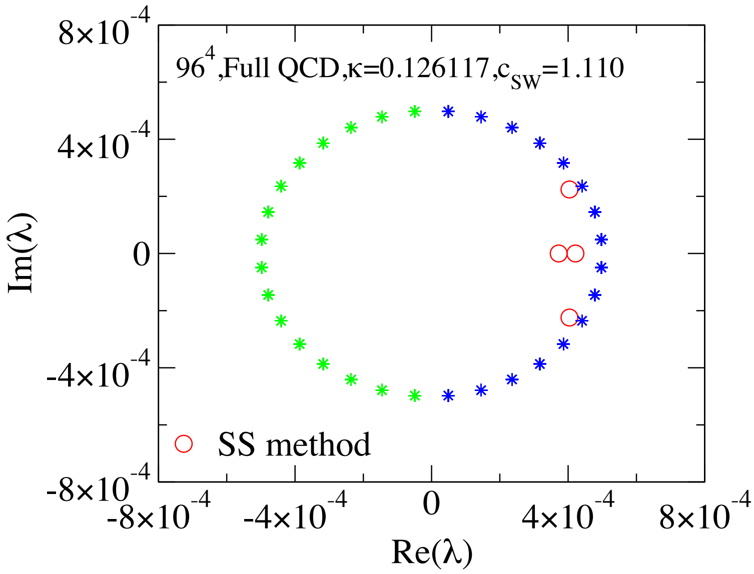

Figure 5.4: Same as Fig. 5.3 for the $O(a)$-improved Wilson-Dirac matrix in 2+1 flavor QCD.

term, it suffers from the numerical sign problem, failure of 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. The tensor network scheme is a promising theoretical and computational framework to overcome these difficulties. So far we have developed the Grassmann version of the tensor renormalization group (GTRG) algorithm in the tensor network scheme, which allows us to deal with the Grassmann variables directly. The GTRG algorithm was successfully applied to the analysis on the phase structure of one-flavor lattice Schwinger model (2D QED) with and without the θ term showing that the algorithm is free from the sign problem and the computational cost is comparable to the bosonic case thanks to the direct manipulation of the Grassmann variables. This was the first successful application of the tensor network scheme to a Euclidean lattice gauge theory including relativistic fermions. Toward the final target of 4D QCD we are currently working on three research subjects in the tensor network scheme: (i) non-Abelian gauge theories, (ii) higher dimensional (3D or 4D) models, and (iii) development of computational techniques for physical observables. Figure 5.5 presents a preliminary result for analysis of the phase transition in the 4D Ising model. The precision of the GTRG algorithm is controlled by the parameter D_{cut}. We observe that the critical (inverse) temperature K_{c} converges close to the previous Monte Carlo result (blue line) as D_{cut} increases. It should be noted that our result is directly obtained on a 1024^4 lattice, while the Monte Carlo result was obtained by extrapolating the data on 80^4 and smaller lattices to the thermodynamic limit.

5.4 Schedule and Future Plan

5.4.1 QCD at finite temperature and finite density

We are now investigating the phase structure in 2+1 flavor QCD with the Kurtosis intersection method and the multi-parameter reweighting method. The first target is to determine the critical end line on the m_{ud}-m_{s} plane. Especially, we are interested in small m_{ud} region.

5.4.2 Nuclei in lattice QCD

So far our study reveals that the dineutron channel is a bound state at heavier quark masses corresponding to $m_\pi \geq 300$ MeV. We currently make a large scale simulation at the physical quark mass. We are also investigating possible sources of the systematic errors.

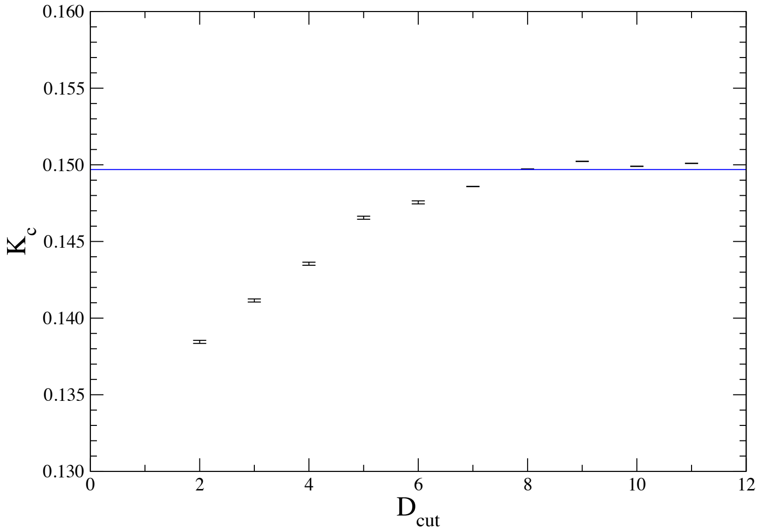

Figure 5.5: D_{cut} dependence of critical (inverse) temperature K_{c} in 4D Ising model on a 1024^4 lattice. Blue line denotes the previous Monte Carlo result.

5.4.3 Development of algorithms and computational techniques

Application of z-Pares to lattice QCD on K computer

In collaboration with Sakurai group at University of Tsukuba we work on an algorithmic improvement to efficiently solve the shifted Wilson-Dirac equation on the discretized contour.

Tensor network scheme in path-integral formalism

We are now try to apply the tensor network scheme to various spin models and non-Abelian lattice gauge theories on higher dimensions. It is also an interesting subject to apply the GTRG method to the chiral fermion.

5.5 Publications

Journal Articles

[1] CSSM and QCDSF-UKQCD Collaborations: A. J. Chambers et al. “Disconnected contributions to the spin of the nucleon”. In: *Physical Review* D92 (2015), p. 114517.

[2] F.-K. Guo et al. “Electric Dipole Moment of the Neutron from 2+1 Flavor Lattice QCD”. In: *Physica Review Letters* 115 (2015), p. 062001.

[3] QCDSF-UKQCD Collaboration: R. Horsley et al. “Lattice determination of Sigma-Lambda mixing”. In: *Physica Review* D91 (2015), p. 074512.

[4] X.-Y. Jin et al. “Curvature of the critical line on the plane of quark chemical potential and pseudoscalar meson mass for three-flavor QCD”. In: *Physical Review* D92 (2015), p. 114511.

[5] Y. Kuramashi et al. “Critical endline of the finite temperature phase transition for 2+1 flavor QCD around the SU(3)-flavor symmetric point”. In: arXiv:1605.04659 [hep-lat] (2016).

[6] CSSM and QCDSF-UKQCD Collaborations: P. E. Shanahan et al. “Charge symmetry violation in the electromagnetic form factors of the nucleon”. In: *Physical Review* D91 (2015), p. 113006.

[7] Eigo Shintani et al. “Neutron and proton electric dipole moments from $N_f = 2+1$ domain-wall fermion lattice QCD”. In: *Physical Review* D93 (2016), p. 094503.

[8] Hiroya Suno. “Geometrical structure of helium triatomic systems: comparison with the neon trimer”. In: *Journal of Physics* B49 (2016), p. 014003.

[9] Takeshi Yamazaki et al. “Study of quark mass dependence of binding energy for light nuclei in 2+1 flavor lattice QCD”. In: *Physical Review* D92 (2015), p. 014501.

Conference Papers

[10] V. G. Bornyakov et al. "Determining the scale in Lattice QCD". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 264.

[11] A. J. Chambers et al. "Applications of the Feynman-Hellmann theorem in hadron structure". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 125.

[12] J. Dragos et al. "Improved determination of hadron matrix elements using the variational method". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 328.

[13] R. Horsley et al. "Improving the lattice axial vector current". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 138.

[14] Renwick J. Hudspith et al. "Determining the QCD coupling from lattice vacuum polarization". In: (LATTICE 2015) (2016), p. 268.

[15] K.-I. Ishikawa et al. "2+1 flavor QCD simulation on a 96^4 lattice". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 075.

[16] K.-I. Ishikawa et al. "Mass and Axial current renormalization in the Schrödinger functional scheme for the RG-improved gauge and the stout smeared $O(a)$-improved Wilson quark actions". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 271.

[17] H. Kobayashi et al. "Optimization of Lattice QCD with CG and multi-shift CG on Intel Xeon Phi Coprocessor". In: *Proceedings of Science* (LATTICE 2015).029 (2016).

[18] Y. Nakamura et al. "Towards the continuum limit of the critical endline of finite temperature QCD". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 160.

[19] Yuya Shimizu and Yoshinobu Kuramashi. "Study of the continuum limit of the Schwinger model using Wilson's lattice formulation". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 049.

[20] Eigo Shintani. "Error reduction using the covariant approximation averaging". In: (EPS-HEP2015) (2015), p. 367.

[21] Eigo Shintani. "Progress of lattice calculation of light-by-light contribution to muon g-2". In: 273-275 (2016), p. 1624.

[22] Eigo Shintani and Hartmut Wittig. "High statistic analysis of nucleon form factors and charges in lattice QCD". In: (LATTICE 2015) (2016), p. 122.

[23] H. Suno et al. "Eigenspectrum calculation of the non-Hermitian $O(a)$-improved Wilson-Dirac operator using the Sakurai-Sugiura method". In: (LATTICE 2015) (2016), p. 026.

[24] S. Takeda et al. "Phase structure of $N_f = 3$ QCD at finite temperature and density by Wilson-Clover fermions". In: *Proceedings of Science* (LATTICE 2015) (2016), p. 145.

[25] Takeshi Yamazaki for PACS Collaboration. "Light Nuclei and Nucleon Form Factors in $N_f = 2 + 1$ Lattice QCD". In: (LATTICE 2015) (2016), p. 081.

Invited Talks

[26] Y. Kuramashi. *Tensor Network Scheme for Lattice Gauge Theories*. XXVII IUPAP Conference on Computational Physics (CCP2015). Indian Institute of Technology Guwahati,, Assam, India, December 2-5, 2015.

[27] Y. Nakamura. *Phase diagram of $N_f = 3$ QCD*. Workshop on 'Physics at finite temperature and density with lattice QCD simulation'. University of Tsukuba, Tsukuba, Japan, September 5, 2015.

[28] Y. Nakamura. *Physics on the post K supercomputer*. International Symposium on Computing Energy Landscape in Material Science and Particles Physics. Kanazawa University, Kanazawa, Japan, February 19-20, 2016.

[29] Y. Nakamura. *The world of elementary particles*. 70th AICS Café. RIKEN AICS, Kobe, Japan, April 17, 2015.

[30] Yuya Shimizu. *Tensor renormalization group approach to (1+1)-dimensional lattice QED*. Workshop on 'Recent progress on DMRG method'. RIKEN AICS, Kobe, Japan, August 25-26, 2015.

[31] Yuya Shimizu. *Tensor Renormalization Group Approach to 2D Lattice QED - as a first step toward lattice QCD -*. Seminar. Tokyo Institute of Technology, Tokyo, Japan, November 19, 2015.

[32] Eigo Shintani. *Electric polarizability and magnetic moment in external electric field*. Workshop on 'High precision QCD at low energy'. Benasque, Spain, August 2-22, 2015.

[33] Eigo Shintani. *Error reduction using the covariant approximation averaging*. EPS-HEP2015. Vienna, Austria, July 22-29, 2015.

[34] Eigo Shintani. *Improved Estimate of Proton Lifetime in lattice QCD*. Brookhaven Forum 2015. Brookhaven National Laboratory, New York, USA, October 7-9, 2015.

[35] Eigo Shintani. *Proton Decay and other BSM in the lattice*. INT Program INT-15-3: Intersections of BSM Phenomenology and QCD for New Physics Searches. Seattle, WA, USA, September 14-October 23, 2015.

[36] Eigo Shintani. *Strong coupling constant from Adler function in lattice QCD*. MITP workshop 'Determination of fundamental parameters in QCD'. Mainz, Germany, March 7-12, 2016.

[37] Eigo Shintani. *Strong coupling constant from vector vacuum polarization function on the lattice*. RBRC Workshop on Lattice Gauge Theories 2016. Brookhaven National Laboratory, New York, USA, March 9-11, 2016.

[38] Hiroya Suno. *Theoretical study of the triple-alpha system in ^{12}C using the hyperspherical slow discretization*. RCNP Colloquium. Osaka University, Osaka, Japan, July 1, 2015.

[39] Takeshi Yamazaki. *Light nuclei and nucleon form factors in $N_f = 2 + 1$ lattice QCD*. The 5th International Workshop on Lattice Hadron Physics (LHPV). Conference Centre of the Cairns Colonial Club Resort, Cairns, Australia, June 20-24, 2015.

[40] Takeshi Yamazaki. *Light nuclei and nucleon form factors in $N_f = 2+1$ lattice QCD*. Long-term and Nishinomiya-Yukawa Memorial International Workshop on 'Computational Advances in Nuclear and Hadron Physics' (CANHP2015). Yukawa Institute of Theoretical Physics (YITP), Kyoto University, Kyoto, Japan, September 21-October 30, 2015.

[41] Takeshi Yamazaki. *Light nuclei from 2+1 flavor lattice QCD*. Workshop on 'Lattice Nuclei Nuclear physics and QCD - Bridging the gap -'. European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*), Torento, Italy, June 6-10, 2015.

[42] Takeshi Yamazaki. *Nucleon form factors and light nuclei in $N_f = 2 + 1$ lattice QCD*. RBRC Workshop on Lattice Gauge Theories 2016. Brookhaven National Laboratory, New York, USA, March 9-11, 2016.

Posters and Presentations

[43] Y. Nakamura. *Towards the continuum limit of the critical endline of finite temperature QCD* (talk). 33rd International Symposium on Lattice Field Theory (Lattice 2015). Kobe International Conference Center, Kobe, Japan, July 14-18, 2015.

[44] Yuya Shimizu. *Study of the continuum limit of the Schwinger model using Wilson's lattice formulation* (talk). 33rd International Symposium on Lattice Field Theory (Lattice 2015). Kobe International Conference Center, Kobe, Japan, July 14-18, 2015.

[45] Eigo Shintani. *High statistic analysis of nucleon form factors and charges in lattice QCD* (talk). 33rd International Symposium on Lattice Field Theory (Lattice 2015). Kobe International Conference Center, Kobe, Japan, July 14-18, 2015.

[46] Hiroya Suno. *Calculation of eigenvalues and eigenvectors for large sparse non-Hermitian matrices in lattice QCD* (talk). 4th Joint Laboratory for Extreme-Scale Computing Workshop. Bonn, Germany, December 2-4, 2015.

[47] Hiroya Suno. *Calculation of the triple-alpha reaction strengths using the hyperspherical slow variable description* (talk). 2015 Autumn Meeting of the Physical Society of Japan. Osaka City University, Osaka, Japan, September 25-28, 2015.

[48] Hiroya Suno. *Eigenspectrum calculation of the non-Hermitian $O(a)$-improved Wilson-Dirac operator using the Sakurai-Sugiura method* (talk). 33rd International Symposium on Lattice Field Theory (Lattice 2015). Kobe International Conference Center, Kobe, Japan, July 14-18, 2015.

[49] Hiroya Suno. *Eigenspectrum calculation of the $O(a)$-improved Wilson-Dirac operator in lattice QCD using the Sakurai-Sugiura method* (poster). International Workshop Workshop on Eigenvalue Problems: Algorithms, Software and Applications, in Petascale Computing (EPASA 2015). Tsukuba, Japan, September 14-16, 2015.

[50] Hiroya Suno. *Eigenspectrum calculation of the O(a)-improved Wilson-Dirac operator in lattice QCD using the Sakurai-Sugiura method* (poster). The 6th AICS International Symposium. RIKEN AICS, Kobe, Japan, February 22-23,, 2016.

[51] Hiroya Suno. *Geometrical structure of helium triatomic systems: comparison with the neon trimer* (poster). Quarks to Universe in Computational Science 2015. Nara, Japan, November 4-8, 2015.

[52] Takeshi Yamazaki. *Calculation of binding energy for light nuclei in $N_f = 2 + 1$ lattice QCD* (talk). 2016 Annual Meeting of the Physical Society of Japan. Tohoku Gakuin University, Miyagi, Japan, March 19-22, 2015.

[53] Takeshi Yamazaki. *Light nuclei and nucleon form factors from lattice QCD* (talk). Symposium on Quarks to Universe in Computational Science (QUCS 2015). Nara Kasugano International Forum IRAKA, Nara, Japan, November 4-8, 2015.

[54] Takeshi Yamazaki. *Light nuclei and nucleon form factors in $N_f = 2 + 1$ lattice QCD* (talk). 33rd International Symposium on Lattice Field Theory (Lattice 2015). Kobe International Conference Center, Kobe, Japan, July 14-18, 2015.

[55] Takeshi Yamazaki. *Pilot study toward nucleus structure calculation with lattice QCD* (poster). HPCI the Second Project Report Meeting. National Museum of Emerging Science and Innovation, Tokyo, Japan, October 26, 2015.

[56] Takeshi Yamazaki. *Study of nucleon form factors in 2+1 flavor QCD with an imporved Wilson fermion action* (talk). 2015 Autumn Meeting of the Physical Society of Japan. Osaka City University, Osaka, Japan, September 25-28, 2015.

[57] Yusuke Yoshimura. *Grassmann tensor renormalization group for the lattice Gross-Neveu model with finite chemical potential* (poster). 33rd International Symposium on Lattice Field Theory (Lattice 2015). Kobe International Conference Center, Kobe, Japan, July 14-18, 2015.