6. Field Theory Research Team

6.1. Team members

Yoshinobu Kuramashi (Team Leader)

Yoshifumi Nakamura (Research Scientist)

Hiroya Suno (Research Scientist, Joint Position with the Nishina Center for Accelerator-based Research)

Xia-Yong Jin (Postdoctoral Researcher)

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Ken-Ichi Ishikawa (Visiting Scientist)

Shinji Takeda (Visiting Scientist)

Takeshi Yamazaki (Visiting Scientist)

6.2. 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.

6.3. Research Results and Achievements

6.3.1. 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. The Monte Carlo simulation technique, which has been successfully applied to the finite temperature phase transition studies in lattice QCD, cannot be directly applied to the finite density case due to the complexity of the quark determinant for finite μ . Recently we investigated the phase of the quark determinant with finite chemical potential in lattice QCD using an analytic method: Employing the winding expansion and the hopping parameter expansion to the logarithm of the determinant, we have shown that the absolute value of the phase has an upper bound that grows with the spatial volume but decreases exponentially with an increase in the temporal extent of the lattice. Based on this analysis we have carried out a finite size scaling study for 4 flavor QCD using the O(a) improved Wilson quark action and the Iwasaki gauge action. This is the first application of the finite size scaling study to the finite density QCD. We choose κ =0.1385 at β =1.58 whose lattice spacing is roughly 0.33 fm. Spatial volume is varied from 6^3 to 10^3 with the temporal size fixed at N_T=4. The transition point is around μ /T～0.5. The left panel of Fig. 1 shows the susceptibility of the quark number as a function of a μ . We observe that the peak height grows as the spatial volume increases. In the right panel of Fig. 1 we plot the spatial volume dependence of the susceptibility peak for various obsevables including the quark number. A clear linear scaling indicates the first order phase transition. These are encouraging results demonstrating that the finite size scaling study is useful even in the finite density QCD.

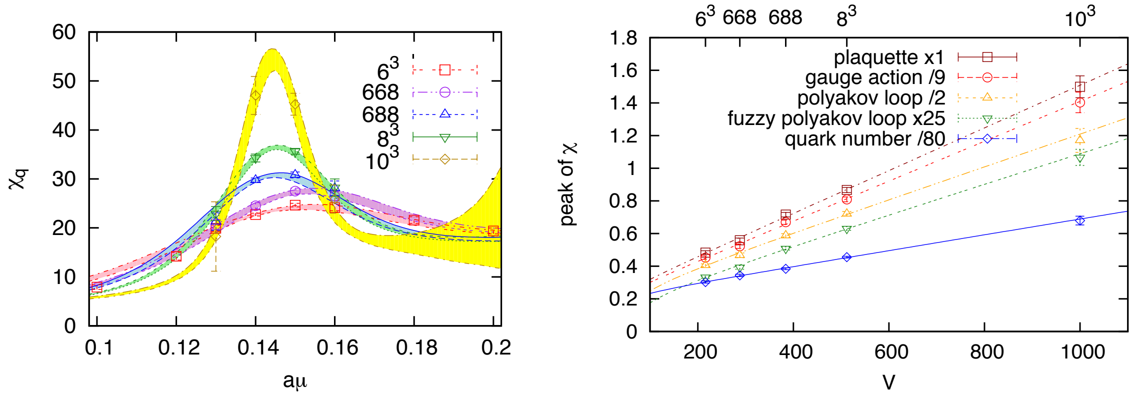
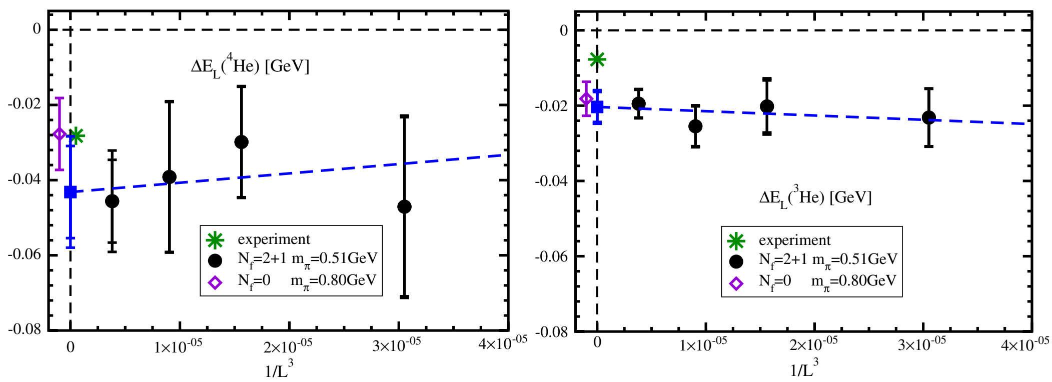


Figure 1: Susceptibility of the quark number as a function of a μ (left) and spatial volume dependence for various observables together with the fit results in the form of $c_1V+c_0+c_{-1}/V$ with V the spatial volume (right).

6.3.2 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. 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 have investigated the dynamical quark effects on the binding energies of the helium nuclei, the deuteron and the dineutron. We perform 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. In Fig. 2 we plot the spatial volume dependence of the energy difference ΔE_L as a function $1/L^3$ with L the spatial extent. A finite energy difference left in the infinite spatial volume limit leads us to the conclusion that the measured ground states for all the channels are bound. We also point out a possibility that the dynamical quark effects might be small at rather heavy quark mass region.



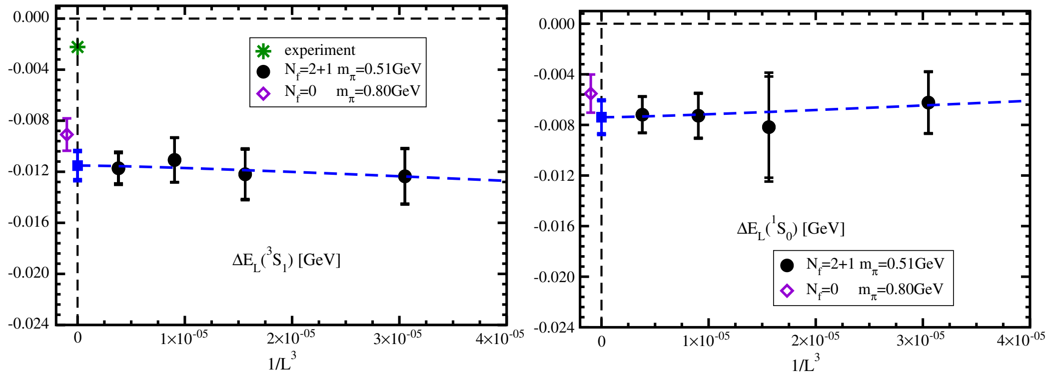


Figure 2: Spatial volume dependence of ΔE_L in GeV units for the ^{4}He (top left), ^{3}He (top right), $^3S_1$ (bottom left) and $^1S_0$ (bottom right) channels. Extrapolated results to the infinite spatial volume limit in 2+1 flavor QCD (blue square) and quenched QCD (violet diamond) are also presented.

6.3.3. Development of algorithms and computational techniques

We consider to solve the linear systems with multiple right-hand sides expressed as AX=B, where A is an N×N matrix and X, B are N×L matrices with L the number of multiple right-hand side vectors. Various fields in computational sciences face this type of problem. In lattice QCD simulations, for example, one of the most time consuming part is to solve the Wilson-Dirac equation with the multiple right-hand sides, where A is an N×N complex sparse non-Hermitian matrix and X, B are N×L complex matrices with N the number of four dimensional space-time sites multiplied by 12. We aim at reducing the computational cost with the block Krylov subspace method which makes convergence faster than the non-blocked method with the aid of better search vectors generated from wider Krylov subspace enlarged by the number of multiple right-hand side vectors. We improve the block BiCGSTAB algorithm with the QR decomposition. After an optimization of the matrix-vector multiplication on K computer, the sustained performance for the block solver has reached nearly 35% of theoretical peak performance.

6.4. Schedule and Future Plan

6.4.1. QCD at finite temperature and finite density

Before exploring the phase structure in 2+1 flavor QCD, we plan to investigate the 3 flavor case with the finite size scaling study. We mainly focus on the location of the critical end line in three dimensional parameter space of the pion mass, chemical potential and temperature.

6.4.2. Nuclei in lattice QCD

The existence of the bound state observed in the $^1S_0$ channel in 2+1 flavor QCD looks odd from the experimental point of view. We expect that the bound state in the $^1S_0$ channel vanishes at some lighter quark mass toward the physical point. To confirm this scenario we are now carrying out a simulation around m_π=300 MeV in 2+1 flavor QCD.

6.4.3. Development of algorithms and computational techniques

We are now ready to check the arithmetic performance and the scalability of the block BiCGSTAB with the QR decomposition optimized on K computer employing a real problem in lattice QCD. We investigate to what extent the cost is reduced thanks to diminished number of iterations and efficient cache usage.

6.5. Publication, Presentation and Deliverables

(1) Journal Papers

1. PACS-CS Collaboration: S. Aoki et al., 1+1+1 Flavor QCD+QED Simulation at the Physical Point", Physical Review D86 (2012) 034507.
2. T. Yamazaki, K.-I. Ishikawa, Y. Kuramashi, A. Ukawa, "Helium nuclei, deuteron and dineutron in 2+1 flavor lattice QCD", Physical Review D86 (2012) 074514.
3. Tuomas Karavirta, Jarno Rantaharju, Kari Rummukainen, Kimmo Tuominen, "Determining the conformal window: SU(2) gauge theory with N_f = 4, 6 and 10 fermion flavours", Journal of High Energy Physics 1205 (2012) 003.

(2) Conference Papers

1. H. Suno, E. Hiyama, M. Kamimura, "Theoretical study of triatomic systems involving helium atoms", (Accepted, talk given at the 20th International IUPAP Conference on Few-Body Problems in Physics (Fukuoka, Japan, August 20-24, 2012)).
2. X.-Y. Jin and R. D. Mawhinney, "Lattice QCD with 12 Quark Flavors: A Careful Scrutiny", (Accepted, talk given at Strong Coupling Gauge Theories in the LHC Perspective (SCGT 12) (Nagoya University, Nagoya, Japan, December 4-7, 2012)).
3. Tuomas Karavirta, Kimmo tuominen, Jarno Rantaharju, Kari Rummukainen, "Mapping the Conformal Window: SU(2) with 4, 6 and 10 flavors of fermions", Proceedings of Science LATTICE2012 (2012) 037.
4. T. Boku, K.-I. Ishikawa, Y. Kuramashi, K. Minami, Y. Nakamura, F. Shoji, D. Takahashi, M. Terai, A. Ukawa, T. Yoshie, "Multi-block/multi-core SSOR preconditioner for the QCD quark solver for K computer", Proceedings of Science (Lattice 2012) 188.
5. T. Yamazaki, K.-I. Ishikawa, Y. Kuramashi, A. Ukawa, "Bound states of multi-nucleon

channels in N_f=2+1 lattice QCD", Proceedings of Science (Lattice 2012) 143.

6. S. Takeda, X-Y. Jin, Y. Kuramashi, Y. Nakamura, A. Ukawa, "Finite size scaling for 4-flavor QCD with finite chemical potential", Proceedings of Science (Lattice 2012) 066.

(3) Invited Talks

1. Yoshinobu Kuramashi, "1+1+1 Flavor QCD+QED Simulation at the Physical Point", New Horizons for Lattice Computations with Chiral Fermions (BNL, New York, USA, May 14-16, 2012).
2. Yoshinobu Kuramashi, "Lattice QCD – From Quarks and Nuclei –", 10th International Meeting on High-Performance Computing for Computational Science (VECPAR2012) (Kobe, Japan, July 17-20, 2012).
3. Yoshifumi Nakamura, "Block Krylov Subspace Method for QCD Simulation", QCDNA VII (University of Adelaide, Adelaide, Australia, July 2-4, 2012).
4. H. Suno, "Efimov effect and resonances in atomic and molecular physics", YITP workshop: Resonances and non-Hermitian systems in quantum mechanics (Kyoto, Japan, December 13-16, 2012).
5. X.-Y. Jin and R. D. Mawhinney, "Lattice QCD with 12 Quark Flavors: A Careful Scrutiny", Strong Coupling Gauge Theories in the LHC Perspective (SCGT 12) (Nagoya University, Nagoya, Japan, December 4-7, 2012).
6. X.-Y. Jin and R. D. Mawhinney, "Exploring the phases of QCD with many flavors", QCD Structure I (Central China Normal University, Wuhan, China, October 7-20, 2012).
7. X.-Y. Jin and R. D. Mawhinney, "Exploring the phases of QCD with many flavors", New Horizons for Lattice Computations with Chiral Fermions (BNL, New York, USA, May 14-16, 2012).
8. Jarno Rantaharju, "Mapping Conformal Field theories on the Lattice", Final Colloquium, International Research Training Group, GRK 881, Paris - Bielefeld - Helsinki (Bielefeld University, Germany, September 12 - 14, 2012).
9. Takeshi Yamazaki, "Light nuclei from quenched lattice QCD", New Horizons for Lattice Computations with Chiral Fermions (Brookhaven National Laboratory, NY, USA, May 14-16, 2012).
10. Takeshi Yamazaki, "Calculation of light nuclei from N_f=2+1 lattice QCD", Lattice Hadron Physics IV (LHP IV) (University of Adelaide, Adelaide, Australia, July 2-4, 2012).
11. Takeshi Yamazaki, "Calculation of light nuclei from N_f=2+1 lattice QCD", Cross over workshop "Particle, nucleus, and Universe" x "New Hadron" (Nagoya University, Nagoya, July 12-13, 2012).
12. Takeshi Yamazaki, "Calculation of light nuclei from lattice QCD", Quarks to Universe in

Computational Science (QUCS 2012) (the Reception Hall in Nara Prefectural New Public Hall, Nara, December 13-16, 2012).

13. Takeshi Yamazaki, "Calculation of light nuclei from N_f=2+1 lattice QCD", HPCI Field 5 meeting (FUJISOFT AKIBA Plaza, Tokyo, March 5-6, 2013).
14. Shinji Takeda, "Complex phase of quark determinant of QCD with finite chemical potential and phase structure of 4-flavor QCD", Tokyo Institute of Technology Theoretical Nuclear Physics group Seminar (Ookayama, Tokyo, September 27, 2012).

(4) Posters and presentations

1. Yoshifumi Nakamura, "Towards high performance Lattice QCD simulations on Exascale computers", SC12 (Salt Lake City, Utah, USA, November 10-16, 2012).
2. Yoshifumi Nakamura, "Towards high performance Lattice QCD simulations on Exascale computers", The 3rd AICS International Symposium (Kobe, Japan, February 28 - March 1, 2013).
3. H. Suno, Y. Nakamura, K.-I. Ishikawa, Y. Kuramashi, "Modified Block BiCGSTAB for Lattice QCD on K Computer", The 3rd AICS International Symposium (Kobe, Japan, February 28 - March 1, 2013).
4. H. Suno, E. Hiyama, M. Kamimura, "Theoretical study of triatomic systems involving helium atoms", The 20th International IUPAP Conference on Few-Body Problems in Physics (Fukuoka, Japan, August 20-24, 2012).
5. H. Suno, E. Hiyama, M. Kamimura, "Theoretical study of triatomic systems involving helium atoms" , The 2012 Annual Meeting of Physical Society of Japan (Yokohama, Japan, September 18-21, 2012).
6. H. Suno, E. Hiyama, "Application of the gaussian expansion method to cold atomic few-body systems" , Quarks to Universe in Computational Science (Nara, Japan, December 13-15, 2012).
7. X.-Y. Jin, S. Takeda, Y. Kuramashi, Y. Nakamura, A. Ukawa, "Studying Quantum Chromodynamics at Finite Temperature and Density", The 3rd AICS International Symposium (Kobe, Japan, February 28 - March 1, 2013).
8. X.-Y. Jin, S. Takeda, Y. Kuramashi, Y. Nakamura, A. Ukawa, "Reweighting and Lee-Yang Zero", The 30th International Symposium on Lattice Field Theory (Cairns Convention Centre, Cairns, Australia, June 24-29, 2012).
9. Jarno Rantaharju, Kari Rummukainen, Kimmo Tuominen, "Running coupling in SU(2) with adjoint fermions", Strong Coupling Gauge Theories in the LHC Perspective (SCGT 12), (Nagoya University, Nagoya, Japan, December 4 - 7, 2012).
10. Jarno Rantaharju, Kari Rummukainen, Kimmo Tuominen, "Running coupling in SU(2) with

adjoint fermions", The 3rd AICS International Symposium (Kobe, Japan, February 28 - March 1, 2013).

11. Takeshi Yamazaki, Y. Kuramashi, A. Ukawa, "Bound states of multi-nucleon channels in N_f=2+1 lattice QCD", The 30th International Symposium on Lattice Field Theory (Lattice 2012) (Cairns Convention Centre, Cairns, Australia, June 24-29, 2012).
12. Takeshi Yamazaki, Y. Kuramashi, A. Ukawa, "Study of multi-nucleon bound states from N_f=2+1 lattice QCD", JPS autumn meeting (Kyoto Sangyo University, Kyoto, September 11-14, 2012).
13. Shinji Takeda, "Finite size scaling for 4-flavor QCD with finite chemical potential", The 30th International Symposium on Lattice Field Theory, Lattice 2012 (Cairns Convention Centere, Cairns, Australia, June 24-29, 2012).
14. Shinji Takeda, "Finite size scaling for 4-flavor QCD with finite chemical potential", New Frontiers in Lattice Gauge Theory (The Galileo Galilei Institute for Theoretical Physics, Florence, Italy, August 28-September 28, 2012).

(5) Patents and Deliverables

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