4. Field Theory Research Team

4.1. Team members

Yoshinobu Kuramashi (Team Leader)

Yoshifumi Nakamura (Research Scientist)

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4.2. 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.

4.3. Research Results and Achievements

4.3.1. QCD at finite temperature and finite density

Establishing the QCD phase diagram spanned by the temperature T and the quark chemical potentialμin 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 finiteμ. We investigate the phase of the quark determinant with finite chemical potential in lattice QCD using both analytic and numerical methods. Applying the winding expansion and the hopping parameter expansion to the logarithm of the determinant, we show 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. This analytic but approximate result is confirmed with a numerical study in 4 flavor QCD in which the phase is calculated exactly. Figure 1 shows histogram of the phaseθat the chemical potential aμ=0.2 with a the lattice spacing on the 63×NT lattice in 4 flavor QCD and NT dependence of the phaseθas a function of μ. We observe that the phase$\theta$is suppressed as the temperature T=1/NT decreases with the chemical potentialμfixed. The winding expansion is useful to study the high density region of the QCD phase diagram at low temperatures.
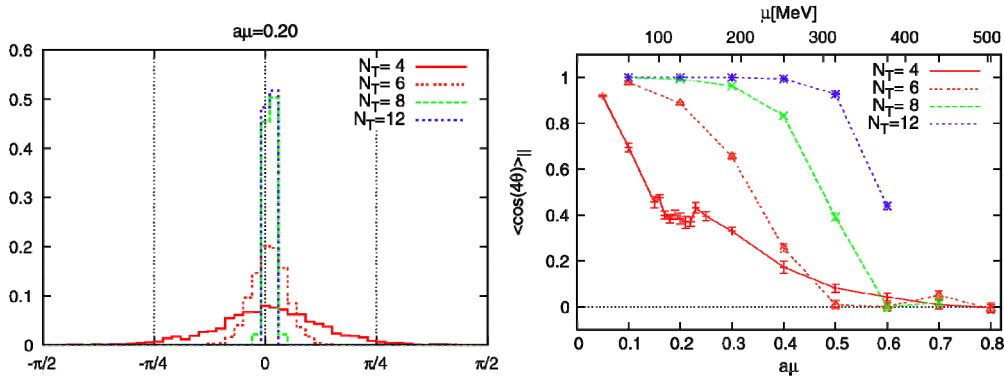

Figure 1. Histogram of the phaseθat the chemical potential $a$$\mu$=0.2 with various N_T (left) and N_T dependence of the phaseθas a function of μ(right).

4.3.2. Nuclei in lattice QCD

In 2010 we succeeded in a direct construction of the 4He and 3He 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 mπ=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 address the issue of bound state in the two-nucleon system at mπ=0.8 GeV in quenched QCD. 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 two-nucleon state by changing the spatial extent of the lattice from 3.1 fm to 12.3 fm. In Fig. 2 we plot the spatial volume dependence of the energy differenceΔEL as a function 1/L3 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 not only spin triplet (3S1) but also singlet (1S0) channels are bound. Furthermore the existence of the bound state is confirmed by investigating the properties of the energy for the first excited state obtained by a 2×2 diagonalization method.
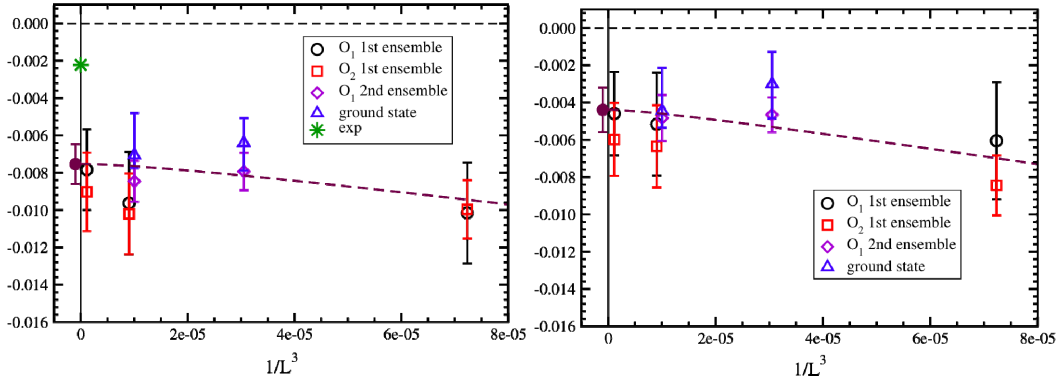

Figure 2. Spatial volume dependence of ΔEL in GeV units for the 3S1 (left) and 1S0 (right) channels. Open symbols represent the results obtained on the L3 boxes employing a couple of alternative calculational methods. Extrapolated results to the infinite spatial volume limit (filled circle) and experimental values (star) are also presented.

4.3.3. 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. Figure 3 shows a representative case for residual norm as a function of number of iterations for the modified block BiCGSTAB. We observe an important feature that the number of iterations required for convergence decreases as the block size L is increased. The numerical results are summarized in Table 1, where the fourth and fifth columns are the number of matrix-vector multiplication (NMVM) and its gain factor, respectively. We find that the gain factor for time is about twice larger than that for NMVM. This is another important advantage of the block methods which allow us an effective usage of cache.
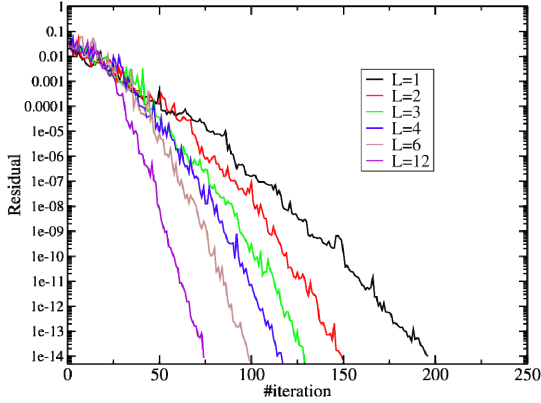

Figure 3. Representative case for residual norm as a function of number of iteration with L=1, 2, 3, 4, 6, 12 on a $32^3 \times 64$ lattice.

Table 1. L dependence for time, gain factor for time, number of matrix-vector multiplication and its gain factor on a $32^3 \times 64$ lattice. Central values are given for gain factors.

$L \times 12/L$	Time [s]	T (gain)	NMVM	NM (gain)
1×12	3827 (755)	1	17 146 (3326)	1
2×6	2066 (224)	1.9	12 942 (1379)	1.3
3×4	1619 (129)	2.4	10 652 (832)	1.6
4×3	1145 (99)	3.3	9343 (835)	1.8
6×2	1040 (87)	3.7	7888 (663)	2.2
12×1	705 (70)	5.4	6106 (633)	2.8

4.4. Schedule and Future Plan

4.4.1. QCD at finite temperature and finite density

Before exploring the phase structure in 2+1 flavor QCD, we plan to investigate the 4 flavor case, where the first order phase transition is confirmed with zero chemical potential and is also expected with the non-zero chemical potential. To pin down the order of the phase transition we have to carry out the finite size scaling analysis by changing the spatial volume systematically.

4.4.2. Nuclei in lattice QCD

The existence of the bound state in the $^1S_0$ channel looks odd from the experimental point of view. However, there are two major systematic errors in our calculation: rather heavy quark mass corresponding to m_π=0.8 GeV and the quenched approximation. We expect that the bound state in the $^1S_0$ channel vanishes at some lighter quark mass with the inclusion of the dynamical quark effects. To confirm this scenario we are now carrying out a simulation of 2+1 flavor QCD with a reduced quark mass.

4.4.3. Development of algorithms and computational techniques

We have demonstrated the effectiveness of the block BiCGSTAB with the QR decomposition: remarkable cost reduction at large L thanks to smaller number of iterations and efficient cache usage. We are going to optimize the code for the K computer and make a numerical test to check the arithmetic performance and the scalability.

4.5. Publication, Presentation and Deliverables

(1)　Journal Papers
　1.　S. Takeda, Y. Kuramashi, A. Ukawa, "Phase of quark determinant in lattice QCD with finite chemical potential", Physical Review D 85 (2012) 096008.
　2.　T. Yamazaki, Y. Kuramashi, A. Ukawa, "Two-nucleon bound states in quenched lattice QCD", Physical Review D 84 (2011) 054506.
　3.　Y. Nakamura, K.-I. Ishikawa, Y. Kuramashi, T. Sakurai, H. Tadano, "Modified block BiCGStab for lattice QCD", Computer Physics Communications 183 (2012) 34.

(2)　Conference Papers
　1.　S. Takeda, Y. Kuramashi, A. Ukawa, "On the phase of quark determinant in lattice QCD with finite chemical potential", Proceedings of Science (Lattice 2011) 144.
　2.　Takeshi Yamazaki for PACS-CS Collaboration, "Bound state of two-nucleon systems in quenched lattice QCD", Proceedings of Science (Lattice 2011) 147.
　3.　Y. Nakamura, K.-I. Ishikawa, Y. Kuramashi, T. Sakurai, H. Tadano, "Modified block BiCGStab for lattice QCD", Proceedings of Science (Lattice 2011) 042.

(3)　Invited Talks
　1.　Yoshinobu Kuramashi, "Nuclei in lattice QCD", Perspective in Nuclear Physics with Large Scale Computing (RIKEN, Wako, Saitama, January 24-25, 2012).

2. Yoshinobu Kuramashi, "Large scale simulations of the femtometer world with lattice QCD", The 4th Forum on Data Engineering and Information Management, deim2012 (Seaside Hotel MAIKO VILLA KOBE, Kobe, March 3-5, 2012).

(4) Posters and presentations

1. Yoshifumi Nakamura, "Modified block BiCGStab for lattice QCD", The XXIX International Symposium on Lattice Field Theory, Lattice 2011 (Squaw Valley, Lake Tahoe, CA, USA, July 11-16, 2011).

2. Yoshifumi Nakamura, "Modified block BiCGStab for lattice QCD", 2nd AICS International Symposium (AICS, Kobe, Hyogo, March 1-2, 2012).

3. Xiao-Yong Jin, "Exploring phases of QCD on the lattice", 2nd AICS International Symposium (AICS, Kobe, Hyogo, March 1-2, 2012).

4. Takeshi Yamazaki, "Bound state of two-nucleon systems in quenched lattice QCD", The XXIX International Symposium on Lattice Field Theory, Lattice 2011 (Squaw Valley, Lake Tahoe, CA, USA, July 11-16, 2011).

5. Takeshi Yamazaki, "Bound state in two-nucleon systems with lattice QCD", The Physics Society in Japan 2011 Fall Meeting (Hirosaki University, Hirosaki, Aomori, September 16-19, 2011).

6. Takeshi Yamazaki, "Bound states of multi-nucleon systems in lattice QCD", 2nd AICS International Symposium (AICS, Kobe, Hyogo, March 1-2, 2012).

7. Takeshi Yamazaki, "Calculation of light nuclei in lattice QCD", HPCI Strategic Program Field 5 "The origin of matter and the universe" Symposium (Akihabara Convention Hall, Akihabara, Tokyo, March 7-8, 2012).

8. Shinji Takeda "Running coupling constant of ten-flavor QCD with the Schrödinger functional method", Symposium on Lattice Gauge Theory (Wuppertal, Germany, May 2, 2011).

9. Shinji Takeda, "On the phase of quark determinant in lattice QCD with finite chemical potential", The XXIX International Symposium on Lattice Field Theory, Lattice 2011 (Squaw Valley, Lake Tahoe, CA, USA, July 11-16, 2011).

10. Shinji Takeda, "Complex phase in QCD with finite chemical potential", Progress of Computational Physics in Particle Physics, Nuclear Physics and Astrophysics (Nemunosato, Mie, December 3-5, 2011).

(5) Patents and Deliverables

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