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 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. 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 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 was the first application of the finite size scaling study to the finite density QCD. After the study of 4 flavor QCD we have moved to 3 flavor case. The main target is to trace the critical end line in the parameter space of temperature, chemical potential and hopping parameter (quark mass). We employ two strategies to determine the critical end point in simulation with fixed chemical potential. One is to identify at which temperature the Binder cumulant/Kurtosis measured at the transition point on two different spatial volumes intersects. This method is based on the property of opposite spatial volume dependence of the Binder cumulant/Kurtosis at the transition point between the first order phase transition side and the crossover one. The other is to locate the critical temperature where a gap of transition point for two observables potentially allowed in the crossover side vanishes. Physical observables are calculated with the phase reweighting method. We evaluate the phase of determinant exactly by developing an efficient numerical technique with the use of a dimensional reduction of temporal direction.

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 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, 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 have to disappear at some quark mass toward the physical value. We are now investigating the quark mass dependence performing a simulation at m_π=0.30 GeV.

3.3. Development of algorithms and computational techniques

3.3.1. Iterative method to solve large system of linear equations

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 for a $12^3\times24$ lattice on 16 nodes. As a next step we have applied the block BiCGSTAB with the QR decomposition to a real problem in lattice QCD. We employ a set of configurations generated at almost the physical point (κ_{ud},κ_s) = (0.126117,0.124790) on 96^4 in 2+1 flavor lattice QCD using the nonperturbatively O(a) improved Wilson quark action with c_{SW}=1.11 and the Iwasaki gauge action at β=1.82. Stout smearing procedure is employed with the parameters N_{stout}=6 and α=0.1. Our numerical test is performed on 2048 nodes on the K computer so that each node has a $12^3\times24$ lattice. Table I shows the *L* dependence of the computational cost to solve the Wilson-Dirac equation. We find that both the number of inner matrix-vector multiplications and the computational time divided by L decrease by about 15% as L increases from 1 to 12.

We have applied the optimization technique acquired in lattice QCD to RSDFT (Real Space Density Functional Theory) which is widely used to calculate ground state energies of the quantum many body states in the condensed matter physics and the nuclear physics. The sustained performance for the matrix-vector multiplication part in the RSDFT code is successfully increased from 3.0% to 8.3%. This work is done in collaboration with Sakurai group at University of Tsukuba who are developing a massively parallel eigenvalue analysis engine for post-petascale machines with a hierarchical parallel structure under a research area of the CREST program "Development of System Software Technologies for post-Peta Scale High Performance Computing".

Table 1: L dependence of the number of inner matrix-vector multiplications (IMVMs) and execution time to solve the Wilson-Dirac equation.

L	#IMVM	time [s]	time/L [s]
1	915.3	65.2	65.2
2	913.0	128.4	64.2
3	876.8	193.8	64.6
4	869.7	235.6	58.9
6	856.5	349.3	58.2
12	770.0	669.0	55.8

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

The Schwinger model, two-dimensional QED, has been used as a theoretical test bed for QCD. It has many QCD-like properties: confinement for fermions, chiral symmetry breaking due to the $U_A(1)$ anomaly, etc. The lattice regularized version of the Schwinger model is also favorable for the development of numerical techniques to tackle lattice QCD. The hybrid Monte Carlo algorithm (HMC) is the most successful method to implement dynamical fermions so far. However, it loses validity when the determinant of the lattice-regularized Dirac matrix can be negative. Such a difficulty has been preventing us from studying the phase structure of the one-flavor lattice Schwinger model in the Wilson fermion formulation with the HMC algorithm. We apply the Grassmann tensor renormalization group to the lattice Schwinger model with one-flavor of the Wilson fermion. We demonstrate that the GTRG works well even at the critical hopping parameter where the negative sign from the fermion determinant may arise, and determines the phase structure of the one-flavor lattice Schwinger model. This is the first application of the GTRG to lattice gauge theory including fermions. Since it has been shown that the GTRG has a strong advantage that it does not suffer from the sign problem caused by the fermion determinant, next step may be an application of the GTRG to the physical system with the so-calledθterm where the action is a complex number. A numerical analysis of the lattice Schwinger model with theθterm is under way.

4. Schedule and Future Plan

4.1. QCD at finite temperature and finite density

After finishing the investigation of 3 flavor QCD, we plan to explore the analysis of the phase structure in 2+1 flavor QCD with the finite size scaling study. We will focus on the determination of the critical surface in the parameter space of temperature, chemical potential and hopping parameters (quark masses).

4.2. Nuclei in lattice QCD

Our preliminary results at m_π=0.30 GeV in 2+1 flavor QCD show that the dineutron channel seems still bound. We plan to make a large scale simulation at or around the physical quark mass.

4.3. Development of algorithms and computational techniques

4.3.1. Iterative method to solve large system of linear equations

As mentioned at the end of Sec. 3.3.1, Sakurai group at University of Tsukuba are developing software packages for massively parallel eigenvalue computation, one of which is z-Pares (short for Complex Moment-based Parallel Eigen-Solvers). In collaboration with his group we try to apply the z-Pares to an eigenvalue analysis of the Wilson-Dirac operator on a 96^4 lattice in 2+1 flavor lattice QCD on K computer.

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

We are now applying the GTRG method to the Schwinger model with theθterm. Once the GTRG method is proved to be efficient even for the complex action, next step is an extension to the SU(3) gauge theory.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] X-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, "Finite size scaling study of N_f=4 finite density QCD on the lattice", Physical Review D88 (2013) 094508.

[2] Yuya Shimizu and Yoshinobu Kuramashi, "Grassmann Tensor Renormalization Group Approach to One-Flavor Lattice Schwinger Model", arXiv:1403.0642 [hep-lat].

[3] H. Suno, E. Hiyama, and M. Kamimura, "Theoretical Study of Triatomic Systems Involving Helium Atoms", Few-Body Systems 54 (2013) 1557.

[4] H. Suno, "A Theoretical Study of Pure and Mixed Spin-Polarized Tritium and Helium Triatomic Systems Using Hyperspherical Coordinates", Few-Body Systems 55 (2014) 229.

(2) Conference Papers

[5] S. Takeda, X-Y. Jin, Y. Kuramashi, Y. Nakamura, and A. Ukawa, "Finite size scaling for 3 and 4-flavor QCD with finite chemical potential", Proceedings of Science (Lattice 2013) 203.

[6] Xiao-Yong Jin, Yoshinobu Kuramashi, Yoshifumi Nakamura, Shinji Takeda, and Akira Ukawa, "Zeros of QCD partition function from finite density lattices", Proceedings of Science (Lattice 2013) 204.

[7] T. Yamazaki, K.-I. Ishikawa, Y. Kuramashi, and A. Ukawa, "Multi-nucleon bound states in N_f=2+1 lattice QCD", Proceedings of Science (Lattice 2013) 230.

[8] R. Horsley, J. Najjar, Y. Nakamura, H. Perlt, D. Pleiter, P.E.L. Rakow, G. Schierholz, A. Schiller, H. Stüben, and J.M. Zanotti, "SU(3) flavour symmetry breaking and charmed states", Proceedings of Science (Lattice 2013) 249.

[9] A.N. Cooke, R. Horsley, Y. Nakamura, D. Pleiter, P.E.L. Rakow, P. Shanahan, G. Schierholz, H. Stüben, and J.M. Zanotti, "SU(3) flavour breaking and baryon structure", Proceedings of Science (Lattice 2013) 278.

[10] R. Horsley, Y. Nakamura, D. Pleiter, P.E.L. Rakow, G. Schierholz, H. Stüben, R.D. Young, and J.M. Zanotti, "Electromagnetic splitting of quark and pseudoscalar meson masses from dynamical QCD + QED", Proceedings of Science (Lattice 2013) 499.

[11] Jarno Rantaharju, "The Gradient Flow Coupling in Minimal Walking Technicolor", Proceedings of Science (Lattice 2013) 084.

(3) Invited Talks

[12] Y. Kuramashi, "Lattice QCD – From Quarks to Nuclei –", University of Tsukuba and Beihang University Collaboration Meeting on Nuclear Physics (University of Tsukuba, Tsukuba, Japan, November 11-12, 2013).

[13] Y. Kuramashi, "Elementary Particle Physics in Future HPC", The 4th AICS International Symposium (RIKEN AICS, Kobe, Japan, December 2-3, 2013).

[14] Y. Kuramashi, "PACS-CS Project and beyond", 新学術領域「素核宇宙融合による計算科学に基づいた重層的物質構造の解明」のまとめと今後を語る研究会 (Narukoonsen, Miyagi, Japan, December 20-21, 2013).

[15] Y. Nakamura, "The critical endpoint in three flavor QCD", Seminar (KEK, Tsukuba, Japan, October 9, 2013).

[16] Y. Nakamura, "The critical endpoint of the finite temperature phase transition in three flavor QCD", Workshop on "Lattice QCD at finite temperature and density" (KEK, Tsukuba, Japan, January 20-22, 2014).

[17] Jarno Rantaharju, "The Gradient Flow Coupling in Technicolor Models", Seminar (Bielefeld University, Bielefeld, Germany, August 13, 2013).

[18] Jarno Rantaharju, "The Gradient Flow Coupling in Technicolor Models", Seminar (University of Helsinki, Department of physics / Helsinki Institute of physics, Helsinki, Finland, August 21, 2013).

[19] Jarno Rantaharju, "Gradient flow coupling schemes in SU(2) with adjoint fermions", JICFuS Mini-workshop on "Gauge theories with many flavors and related topics" (YITP, Kyoto, Japan, March 10, 2013).

[20] Yuya Shimizu, "Analysis of Two-Dimensional Lattice QED in Theta Vacuum using Tensor Renormalization Group", Seminar (Kanazawa University, Kanazawa, Japan, November 15, 2013).

[21] T. Yamazaki, "Calculation of light nuclei in N_f=2+1 lattice QCD", HPCI Field 5 meeting (FUJISOFT AKIBA Plaza, Tokyo, March 3-4, 2014).

[22] Shinji Takeda, "Exploring QCD phase diagram by Wilson type fermions", German-Japanese Seminar (Regensburg, Germany, November 6, 2013).

[23] Shinji Takeda, "Phase structure of finite density QCD", Workshop on "Lattice QCD at finite temperature and density" (KEK, Tsukuba, Japan, January 20-22, 2014).

(4) Posters and Presentations

[24] Y. Kuramashi, "2+1 Flavor Lattice QCD Simulation on K Computer", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[25] Y. Nakamura, "The critical endpoint of the finite temperature phase transition for three flavor QCD with clover type fermions", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[26] Y. Nakamura, "Towards high performance Lattice QCD simulations on Exascale computers", The International Conference for High Performance Computing, Networking, Storage and Analysis (SC13) (Denver, CO, USA, November 17-22, 2013).

[27] H. Suno, Y. Nakamura, K.-I. Ishikawa, and Y. Kuramashi, "Block BiCGSTAB for lattice QCD on

the K computer", The 4th AICS International Symposium (RIKEN AICS, Kobe, Japan, December 2-3, 2013).

[28] H. Suno, "Theoretical study of weakly bound triatomic systems", JPS 2014 Annual Meeting (Tokai University, Hiratsuka, Japan, March 27-30, 2014).

[29] Xiao-Yong Jin, Yoshinobu Kuramashi, Yoshifumi Nakamura, Shinji Takeda, and Akira Ukawa, "Results from combining ensembles at several values of chemical potential", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[30] Jarno Rantaharju, "The Gradient Flow Coupling in Minimal Walking Technicolor", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[31] Jarno Rantaharju, "The Gradient Flow and the Running Coupling", Sakata Memorial KMI Mini-Workshop on "Strong Coupling Gauge Theories Beyond the Standard Model" (SCGT14Mini) (Nagoya University, Nagoya, Japan, March 5-7, 2014).

[32] Yuya Shimizu, "An Application of Grassmann Tensor Renormalization Group to Low Dimensional Lattice Gauge Theory", JPS 2014 Annual Meeting (Tokai University, Hiratsuka, Japan, March 27-30, 2014).

[33] Shinji Takeda, "Finite size scaling for 3 and 4-flavor QCD with finite chemical potential", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[34] Shinji Takeda, "Exploring finite density QCD with Nf=3 and 4 by Wilson type fermions", The 11th XQCD 2013 (Bern University, Bern, Switzerland, August 5-7, 2013).