Subnuclear System Research Division
RIKEN BNL Research Center
Computing Group

1. Abstract

The computing group founded in 2011 as a part of the RIKEN BNL Research Center established at Brookhaven National Laboratory in New York, USA, and dedicated to conduct researches and developments for large-scale physics computations important for particle and nuclear physics. The group was forked from the RBRC Theory Group.

The main mission of the group is to provide important numerical information that is indispensable for theoretical interpretation of experimental data from the first principle theories of particle and nuclear physics. Their primary area of research is lattice quantum chromodynamics (QCD), which describes the sub-atomic structures of hadrons, which allow us the ab-initio investigation for strongly interacting quantum field theories beyond perturbative analysis.

The RBRC group and its collaborators have emphasized the necessity and importance of precision calculations, which will precisely check the current understandings of nature, and will have a potential to find a physics beyond the current standard model of fundamental physics. We have therefore adopted techniques that aim to control and reduce any systematic errors. This approach has yielded many reliable results.

The areas of the major activities are R&D for high performance computers, developments for computing algorithms, and researches of particle, nuclear, and lattice theories. Since the inception of RBRC, many breakthroughs and pioneering works has carried out in computational forefronts. These are the use of the domain-wall fermions, which preserve chiral symmetry, a key symmetry for understanding nature of particle nuclear physics, the three generations of QCD devoted supercomputers, pioneering works for QCD calculation for Cabibbo-Kobayashi-Maskawa theory, QCD + QED simulation for isospin breaking, novel algorithm for error reduction in general lattice calculation. Now the chiral quark simulation is performed at the physical up, down quark mass, the precision for many basic quantities reached to accuracy of sub-percent, and the group is aiming for further important and challenging calculations, such as the full and complete calculation of CP violating $K \to \pi\pi$ decay and ε'/ε, or hadronic contributions to muon's anomalous magnetic moment $g-2$. Another focus area is the nucleon's shape, structures, and the motion of quarks and gluon inside nucleon called parton distribution, which provide theoretical guidance to physics for sPHENIX and future Electron Ion Collider (EIC), Hyper Kamiokande, DUNE, or the origin of the current matter rich universe (rather than anti-matter). Towards finite density QCD, they also explore Quantum Computing to overcome the sign problem. The Machine Learning (ML) and Artificial Intelligence (AI) are the new topics some of members are enthusiastically studying lately.

2. Major Research Subjects

(1) Search for new law of physics through tests for Standard Model of particle and nuclear physics, especially in the framework of the Cabibbo-Kobayashi-Maskawa (CKM), hadronic contributions to the muon's anomalous magnetic moment $(g-2)$ for FNAL and J-PARC's experiments, as well as B physics at Belle II and LHCb.

(2) Nuclear Physics and dynamics of QCD or related theories, including study for the structures of nucleons related to physics for Electron Ion Collider (EIC or eRHIC), Hyper Kamiokande, T2K, DUNE.

(3) Theoretical and algorithmic development for lattice field theories, QCD machine (co-)design and code optimization.

3. Summary of Research Activity

In 2011, QCD with Chiral Quarks (QCDCQ), a third-generation lattice QCD computer that is a pre-commercial version of IBM's Blue Gene/Q, was installed as an in-house computing resource at the RBRC. The computer was developed by collaboration among RBRC, Columbia University, the University of Edinburgh, and IBM. Two racks of QCDCQ having a peak computing power of 2×200 TFLOPS are in operation at the RBRC. In addition to the RBRC machine, one rack of QCDCQ is owned by BNL for wider use for scientific computing. In 2013, 1/2 rack of Blue Gene/Q is also installed by US-wide lattice QCD collaboration, USQCD. The group has also used the IBM Blue Gene supercomputers located at Argonne National Laboratory and BNL (NY Blue), and Hokusai and RICC, the super computers at RIKEN (Japan), Fermi National Accelerator Laboratory, the Jefferson Lab, and others. From 2016, the group started to use the institutional cluster both GPU and Intel Knight Landing (KNL) clusters installed at BNL and University of Tokyo extensively.

Such computing power enables the group to perform precise calculations using up, down, and strange quark flavors with proper handling of the important symmetry, called chiral symmetry, that quarks have. The group and its collaborators carried out the first calculation for the direct breaking of CP (Charge Parity) symmetry in the hadronic K meson decay ($K \to \pi\pi$) amplitudes, ε'/ε, which provide a new information to CKM paradigm and its beyond. They also provide the hadronic contribution in muon's anomalous magnetic moment $(g-2)_\mu$. These calculation for ε'/ε, hadronic light-by-light of $(g-2)$, are long waited calculation in theoretical physics delivered for the first time by the group. The $K \to \pi\pi$ result in terms of ε'/ε currently has a large error, and deviates from experimental results by 2.1σ. To collect more information to decide whether this deviation is from the unknown new physics or not, the group continues to improve the calculation in various way to reduce their error. Hadronic light-by-light contribution to $(g-2)_\mu$ is improved by more than two order of magnitudes compared to our previous results. As of 2019 summer, their calculation is among the most precise determination for the $g-2$ hadronic vacuum polarization (HVP), and only one calculation in the world for the hadronic light-by-light (HLbL) contribution at physical point. These $(g-2)_\mu$ calculations provide the first principle theoretical prediction for on-going new experiment at FNAL and also for the planned experiment at J-PARC. Other projects including flavor physics in the framework of the

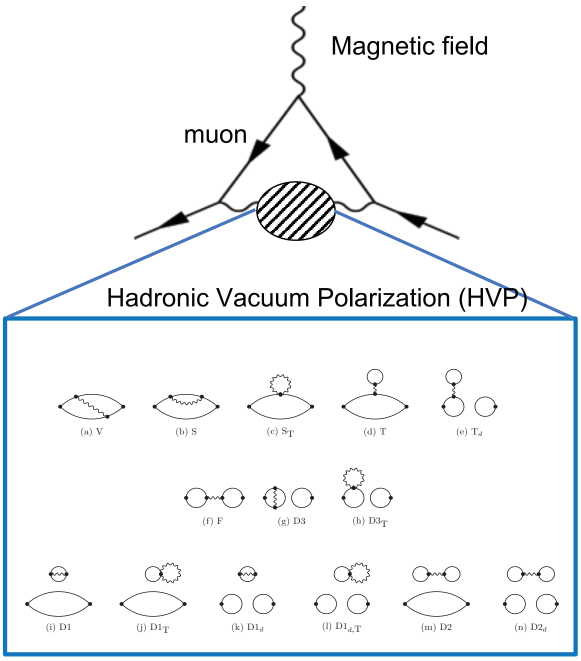

Fig. 1. Feynman diagrams for Lattice QCD computations of Muon's anomalous magnetic moment $(g-2)_\mu$ to take into account for the effects of quark's electric charges. Each diagram, in which the black dots connecting the quark propagators (solid curves) are the electric current emmitting or absorbing photons (wave curves), represents a part of the isospin breaking effects to hadronic vacuum polarization contribution to $(g-2)_\mu$ (top plot).

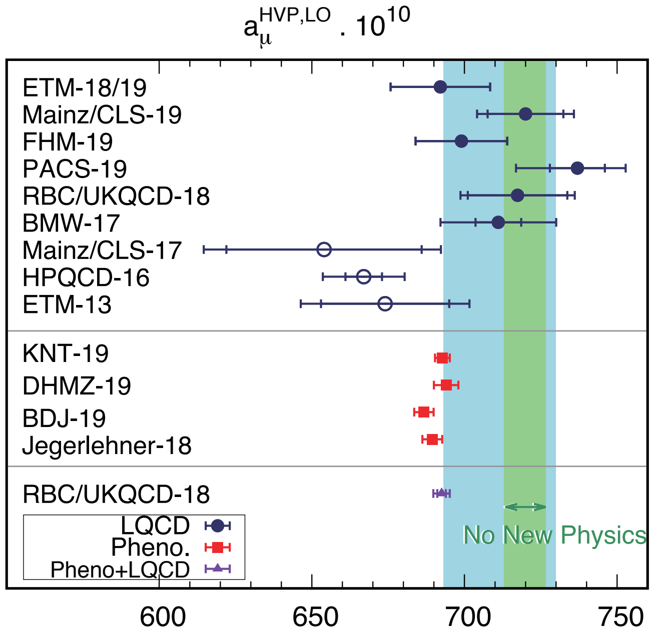

Fig. 2. Current summary of the Hadronic Vacuum Polarization (HVP) contribution for Muon's anomalous magnetic moment $(g-2)_\mu$. Above the upper horizontal line shows various Lattice QCD determinations of HVP while the red results from hadronic decay of electron positron scattering (R-ratio), the green bands is the experimental results of $(g-2)_\mu$ showing a 3–4σ discrepancies.

CKM theory for kaons and B mesons that include the new calculation of b-baryon decay, $\Lambda_b \to p$; the electromagnetic properties of hadrons; the proton's and neutron's form factors and structure function including electric dipole moments; proton decay; nucleon form factors, which are related to the proton spin problem or neutrino-nucleon interaction; Neutron-antineutron oscillations; inclusive hadronic decay of τ leptons; nonperturbative studies for beyond standard model such composite Higgs or dark matter models from strong strongly interacting gauge theories; a few-body nuclear physics and their electromagnetic properties; QCD thermodynamics in finite temperature/density systems such as those produced in heavy-ion collisions at the Relativistic Heavy Ion Collider; Quantum Information, Quantum Computing; and applications of Machine Learning (ML) in field theories.

The RBRC group and its collaborators have emphasized the necessity and importance of precision calculations, which will provide stringent checks for the current understandings of nature, and will have a potential to find physics beyond the current standard model of fundamental physics. We have therefore adopted techniques that aim to control and reduce any systematic errors. This approach has yielded many reliable results, many of basic quantities are now computed within sub-percent accuracies.

The group also delivers several algorithmic breakthroughs, which speed up generic lattice gauge theory computation. These novel technique divides the whole calculation into frequent approximated calculations, and infrequent expensive and accurate calculation using lattice symmetries called All Mode Averaging (AMA), or a compression for memory needs by exploiting the local-coherence of QCD dynamics. Together with another formalism, zMobius fermion, which approximate chiral lattice quark action efficiently, the typical calculation is now improved by a couple of orders of magnitudes, and more than an order of magnitude less memory needs compared to the traditional methods. RBRC group and its collaborators also provide very efficient and generic code optimized to the state-of-arts CPU or GPU, and also improve how to efficiently generate QCD ensemble.

Members

Group Leader

Taku IZUBUCHI

Special Postdoctoral Researchers

Akio TOMIYA

RBRC Researchers

Sergey SYRITSYN
Luchang JIN

Visiting Scientists

Thomas BLUM (Univ. of Connecticut)
Meifeng LIN (BNL)
Chulwoo JUNG (BNL)
Robert MAWHINNEY (Columbia Univ.)
Shigemi OHTA (KEK)
Hiroshi OKI (Nara Women's Univ.)
Tomomi ISHIKAWA (Shanghai Jiao-Tong Univ.)
Christopher KELLY (Columbia Univ.)
Christoph LEHNER (BNL)

List of Publications & Presentations

Publications

[Original Papers]

M. Abramczyk, T. Blum, T. Izubuchi, C. Jung, M. Lin, A. Lytle, S. Ohta, E. Shintani, "Nucleon mass and isovector couplings in 2 + 1-flavor dynamical domain-wall lattice QCD near physical mass," Phys. Rev. D **101**, no.3, 034510 (2020).

T. Izubuchi, L. Jin, C. Kallidonis, N. Karthik, S. Mukherjee, P. Petreczky, C. Shugert, S. Syritsyn, "Valence parton distribution function of pion from fine lattice," Phys. Rev. D **100**, 034516 (2019).

N. H. Christ, X. Feng, L. C. Jin, C. T. Sachrajda, "Finite-volume effects in long-distance processes with massless leptonic propagators," Phys. Rev. D **103**, 014507 (2021).

Y. Li, S. C. Xia, X. Feng, L. C. Jin, C. Liu, "Field sparsening for the construction of the correlation functions in lattice QCD," Phys. Rev. D **103**, 014514 (2021).

C. Y. Seng, X. Feng, M. Gorchtein, L. C. Jin, U. G. Meißner, "New method for calculating electromagnetic effects in semileptonic beta-decays of mesons," J. High Energy Phys. **10**, 179 (2020).

X. Gao, L. Jin, C. Kallidonis, N. Karthik, S. Mukherjee, P. Petreczky, C. Shugert, S. Syritsyn, Y. Zhao, "Valence parton distribution of the pion from lattice QCD: Approaching the continuum limit," Phys. Rev. D **102**, 094513 (2020).

X. Feng, L. C. Jin, Z. Y. Wang, Z. Zhang, "Finite-volume formalism in the $2 \xrightarrow{H_I+H_I} 2$ transition: An application to the lattice QCD calculation of double beta decays," Phys. Rev. D **103**, 034508 (2021).

R. Abdul Khalek *et al.*, "Science Requirements and Detector Concepts for the Electron-Ion Collider: EIC Yellow Report," arXiv:2103.05419 [physics.ins-det].

X. Gao, N. Karthik, S. Mukherjee, P. Petreczky, S. Syritsyn, Y. Zhao, "Pion form factor and charge radius from Lattice QCD at physical point," arXiv:2102.06047 [hep-lat].

X. Gao, N. Karthik, S. Mukherjee, P. Petreczky, S. Syritsyn, Y. Zhao, "Towards studying the structural differences between the pion and its radial excitation," Phys. Rev. D **103**, 094510 (2021).

G. Silvi, S. Paul, C. Alexandrou, S. Krieg, L. Leskovec, *et al.*, "P-wave nucleon-pion scattering amplitude in the $\Delta(1232)$ channel from lattice QCD," Phys. Rev. D **103**, 094508 (2021).

M. Yu. Barabanov, M. A. Bedolla, W. K. Brooks, G. D. Cates, C. Chen, *et al.*, "Diquark correlations in hadron physics: Origin, impact and evidence," Prog. Part. Nucl. Phys. **116**, 103835 (2021).

M. Engelhardt, J. R. Green, N. Hasan, S. Krieg, S. Meinel, J. Negele, A. Pochinsky, S .Syritsyn, "From Ji to Jaffe-Manohar orbital angular momentum in lattice QCD using a direct derivative method," Phys. Rev. D **102**, 074505 (2020).

G. Rendon, L. Leskovec, S. Meinel, J. Negele, S. Paul, *et al.*, "$I = 1/2$ S-wave and P-wave $K\pi$ scattering and the κ and K^* resonances from lattice QCD," Phys. Rev. D **102**, 114520 (2020).

Z. Fan, X. Gao, R. Li, H. -W. Lin, N. Karthik, *et al.*, "Isovector parton distribution functions of the proton on a superfine lattice," Phys. Rev. D **102**, 074504 (2020).

H. T. Ding, S. T. Li, Swagato Mukherjee, A. Tomiya, X. D. Wang, Y. Zhang, "Correlated Dirac eigenvalues and axial anomaly in chiral symmetric QCD," Phys. Rev. Lett. **126**, 082001 (2021).

M. Kawaguchi, S. Matsuzaki, A. Tomiya, "Nonperturbative flavor breaking in topological susceptibility at hot QCD criticality," Phys. Lett. B **813**, 136044 (2021).

H. -T. Ding, C. Schmidt, A. Tomiya, X. -D. Wang, "Chiral phase structure of three flavor QCD in a background magnetic field," Phys. Rev. D **102**, 054505 (2020).

B. Chakraborty, M. Honda, T. Izubuchi, Y. Kikuchi and A. Tomiya, "Digital quantum simulation of the Schwinger model with topological term via adiabatic state preparation," arXiv:2001.00485 [hep-lat].

[Review Articles]

T. Aoyama, N. Asmussen, M. Benayoun, J. Bijnens, T. Blum, M. Bruno, I. Caprini, C. M. Carloni Calame, M. Cè and G. Colangelo, *et al.*, "The anomalous magnetic moment of the muon in the Standard Model," Phys. Rept. **887**, 1–166 (2020).

[Books]

Akio Tomiya, "An introduction to machine learning in physics" (in Japanese), Kodansha, March 2021.

K. Hashimoto, A. Tanaka, A. Tomiya, "Deep learning and physics," Springer, February 2021.

[Proceedings]

T. Izubuchi, H. Ohki and S. Syritsyn, “Computing Nucleon Electric Dipole Moment from lattice QCD,” PoS **LATTICE2019**, 290 (2020).

M. Bruno, T. Izubuchi, C. Lehner and A. S. Meyer, “Exclusive Channel Study of the Muon HVP,” PoS **LATTICE2019**, 239 (2019)

M. Kawaguchi, S. Matsuzaki, A. Tomiya, “Analysis on nonperturbative flavor violation at chiral crossovercriticality in QCD,” arXiv:2005.07003 [hep-ph].

A. Tomiya, Y. Nagai, “Gauge covariant neural network for 4 dimensional non-abelian gaugetheory,” arXiv:2103.11965 [hep-lat].

M. Kawaguchi, S. Matsuzaki, A. Tomiya, “A new critical endpoint in thermomagnetic QCD,” arXiv:2102.05294 [hep-ph].

Y. Nagai, A. Tanaka, A. Tomiya, “Self-learning Monte-Carlo for non-abelian gauge theory withdynamical fermions,” arXiv:2010.11900 [hep-lat].

H. -T. Ding, S. -T. Li, A. Tomiya, X. -D. Wang, Y. Zhang, “Chiral properties of $(2+1)$-flavor QCD in strong magnetic fields at zerotemperature,” arXiv:2008.00493 [hep-lat].

H. -T. Ding, S. -T. Li, S. Mukherjee, A. Tomiya, X. -D. Wang, “Meson masses in external magnetic fields with HISQ fermions,” arXiv:2001.05322 [hep-lat].

Presentations

[International Conferences/Workshops]

L. Jin (invited), “Lattice calculations in muon $g-2$,” The Hadron Mass and Structure Forum, online, April 2021.

L. Jin (invited), “Muon $g-2$: hadronic light-by-light contribution and lattice QCD,” The Muon $g-2$ Discussion Forum, Peking University, online, April 2021.

L. Jin (invited), “Pion electric polarizability,” the χQCD Collaboration Meeting, online, January 2021.

L. Jin (invited), “Lattice calculation of the hadronic light-by-light contribution to the muon magnetic moment,” The Hadron Physics Online Forum, online, August 2020.

S. Syritsyn (invited), “Nucleon Form Factors at High Momentum Transfer from Lattice QCD,” Nuclear & Particle Theory Seminar, MIT/CTP, March 9, 2020.

A. Tomiya (oral), “Self-learning Monte-Carlo for non-abelian gauge theory withdynamical fermions,” APS April Meeting 2020, Virtual, April 18–21, 2020

A. Tomiya (invited), “Self-learning Monte-Carlo for non-abelian gauge theory with dynamical fermions,” Workshop on Non-Equilibrium Systems and Machine Learning, Virtual, March 30, 2020.

A. Tomiya (oral), “Quantum computing for QCD phase diagram? Finite chemicalpotential and temperature?” Kickoff Meeting of C2QA Center, Virtual (BNL), October 30, 2020.

A. Tomiya (invited), “Machine learning and theoretical physics,” Progress of Particle Physics 2020, Virtual (YITP), September 4, 2020.

A. Tomiya (oral), “Thermal field theory with pure states,” Asia-Pacific Symposium for Lattice Field Theory (APLAT 2020), Virtual (KEK), August 6, 2020 (JST).

A. Tomiya (invited), “Applications of machine learning to computational physics,” A. I. for Nuclear Physics, Virginia (Jefferson Laboratory), U.S.A., March 3, 2020.

[Domestic Conferences/Workshops]

富谷昭夫 (口頭発表), “Gauge covariant neural network for 4 dimensional non-abelian gaugetheory,”「ゲージ共変なニューラルネットと 4 次元非可換ゲージ理論への応用 (Gauge covariant neural network for 4 dimensional non-abelian gauge theory)」, Deep Learning and Physics, オンライン開催, 2020 年 4 月 8 日 (JST).

富谷昭夫 (口頭発表),「動的フェルミオンを含む非可換ゲージ理論のための自己学習モンテカルロ法」, 日本物学会第 76 回年次大会, オンライン開催, 2021 年 3 月 12–15 日 (JST).

富谷昭夫 (招待講演), チュートリアル講演「理論物理学における機械学習の応用」, 第 5 回 統計・機械学習若手シンポジウム, オンライン開催, 2020 年 12 月 3–5 日 (JST).

富谷昭夫 (口頭発表),「ニューラルネットを使った 2 次元イジング模型の相検出」, Deep Learning and Physics 2020, オンライン開催 (大阪大学), 2020 年 11 月 26 日 (JST).

[Seminars]

L. Jin (invited), “Lattice calculations in muon $g-2$,” The Theory Seminar at the Department of Physics and Astronomy, University of California, Davis, online, May 2021.

L. Jin (invited), “Lattice calculations in muon $g-2$,” The Lunch Seminar at the Institute of Theoretical Physics, Chinese Academy of Sciences, online, April 2021.

L. Jin (invited), “First-principles calculation of electroweak box diagrams from lattice QCD,” The Physics Seminar in Hunan University, online, December 2020.

L. Jin (invited), “First-principles calculation of electroweak box diagrams from lattice QCD,” The Theory Seminar at the Institute of Modern Physics, Chinese Academy of Sciences, online, July 2020.

L. Jin (invited), “First-principles calculation of electroweak box diagrams from lattice QCD,” The BNL Nuclear Theory Seminar, online, May 2020.

L. Jin (invited), “Lattice calculation of the hadronic light-by-light contribution to the muon magnetic moment,” The QCD Seminar, online, May 2020.

S. Syritsyn (invited), “From quarks and gluons to nucleons and nuclei,” Seminar at IACS (Inst. Adv. Comp. Sci), Stony Brook, Oct 8, 2020.

A. Tomiya (oral), “Gauge covariant neural network for 4 dimensional non-abelian gaugetheory,” MIT, online, April 29, 2020.

A. Tomiya (oral), “Applications of machine learning on theoretical physics,” Ochanomizu University, online, May 19, 2020.

A. Tomiya (oral), “Gauge covariant neural network for 4 dimensional non-abelian gaugetheory,” RIKEN Center for Computational Science (R-CCS), online, April 28, 2020.

A. Tomiya (oral), “Applications of machine learning for theoretical physics,” J-PARC, online, March 18, 2020.

A. Tomiya (oral), “Self-learning Monte-Carlo for non-abelian gauge theory withdynamical fermions,” Yukawa Institute for Theoretical Physics (YITP), Kyoto Univeristy, online, December 7, 2020.

A. Tomiya (oral), “Applications of machine learning on theoretical physics,” Shimane University, online, October 29, 2020

A. Tomiya (oral), “Lattice gauge theory with quantum computers,” RIKEN Center for Computational Science (R-CCS), online, June 3, 2020.

A. Tomiya (oral), “Lattice gauge theory with quantum computers,” Osaka University, online, May 12, 2020.

Awards

富谷昭夫, 理研基礎科学特別研究員 成果発表会ポスター賞, 2021 年 1 月.

Press Releases

Brookhaven National Laboratory (April 7, 2021), “Background on Brookhaven Lab’s Involvement in the Muon g-2 Experiment,” https://www.bnl.gov/newsroom/news.php?a=218814.

CERN Courier (April 14, 2021), “An anomalous moment for the muon,” https://cerncourier.com/a/an-anomalous-moment-for-the-muon/.

UConn Today (May 20, 2021), “UConn Physicists Focus on a Law-Breaking Particle,” https://today.uconn.edu/2021/05/uconn-physicists-focus-on-a-law-breaking-particle/.