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 high energy particle and nuclearphysics. 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 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. The first-principle studies also elucid intrecate nature of various phenomena in quantitive and unambiguous manners. 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 computing codes, 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 dynamics of subnuclear elementary particle quark, the three generations of QCD devoted supercomputers and very efficient software library for lattice gauge theories, pioneering works for QCD calculation for Cabibbo-Kobayashi-Maskawa theory, QCD + QED simulation for isospin breaking, novel algorithms for statistical error reduction in general lattice calculation *etc.* The chiral quark simulation has been performed in a uncompromised setup at the physical up, down quark mass, the precision for many basic quantities reached to accuracy of sub-percent, and the group is working 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 $g - 2$.

Recent focus area is stusies of 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. Closely related calculation has been carried out for the origin of the current matter rich universe (rather than anti-matter). Towards finite density QCD, they also explored Quantum Computing for field theories. Applications of the Machine Learning (ML) and Artificial Intelligence (AI) for novel and more efficient ways to carry out lattice QCD calculations are among the new topics of the group.

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 sPHENIX, Electron Ion Collider (EIC or eRHIC), Hyper Kamiokande, T2K, DUNE, or the matter rich universe

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

3. Summary of Research Activity

Research activities during the current report period by RBRC members include various nulcleon formfactor and structure calculations, hadronic contributions to the anomalous magnetic moment $(g - 2)_\mu$, kaon and B meson physics, and algorithm & software developments.

In April 2020, $(g - 2)_\mu$ experiment collaboration at FNAL carried out a very precise measurement of precession rate of muons under magnetic field to 0.14 parts per million accuracy. This provides a very stringent test of the current understanding of elementary particle physics so called the Standard Model of particle physics. The strong interaction of quark and gluon is described by Quantum Chromo Dyanics (QCD) and is a dominant source of uncertainty in the theoretical prediction of $(g - 2)_\mu$. Members of RBRC has been working on the two separate mode of QCD contributions, Hadronic Vacuum Polarization (HVP) and Hadronic Light-by-Light (HLbL). This year, an update of HVP was reported with an improved precision by adding calculation on the finner space-time lattice to remove systematic error due to non-zero lattice spacing. The quantities are not yet the final total conribution for $(g - 2)_\mu$ but a large part of QCD contributionfrom intermediate energies scale, roughly 200 MeV–1 GeV. The new results of HVP contribution turned out significantly larger than our previous results and consistent with other lattice QCD calcuation by other groups, which emphasis the importance and difficulty of removing lattice spacing error. No an interesting observation is our new value (and other lattice QCD values) has about 4+σ tention to the HVP prediction from hadronic cross section in electron-position collision. It is important to note this is still a comparison of the partial HVP contribution from the intemediate energy region, and the final total HVP contribution including other energies as well as the other systematic effects is ongoing to updated with greater precision soon.

This is only a selected research highlight of members of RBRC this year among other various researches: Machine Learning

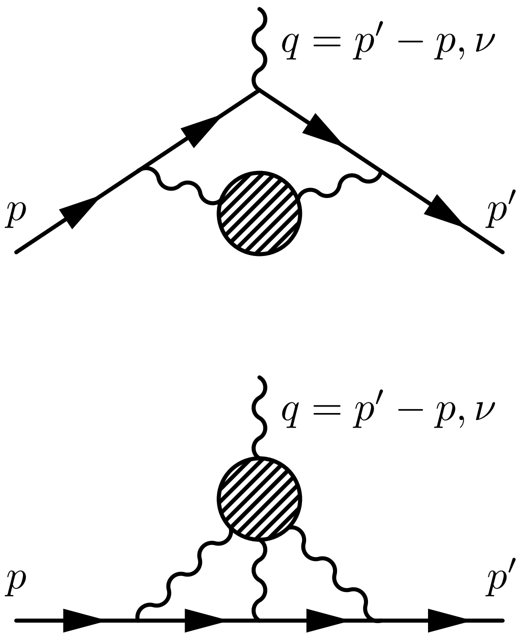

Fig. 1. Feynman diagrams for Lattice QCD computations of Muon's anomalous magnetic moment $(g-2)_\mu$. Hadronic Vaccum Polarization contribution (Left) and Hadronic Light-by-Light contribution (Right).

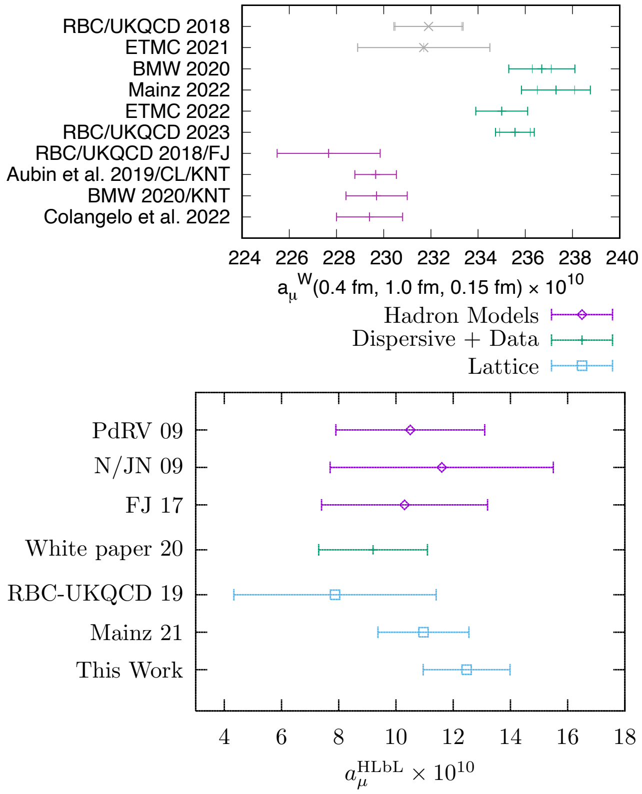

Fig. 2. Current summary of the Hadronic Light-by-Light contribution (HLbL) contribution for Muon's anomalous magnetic moment $(g-2)_\mu$. Above the upper horizontal line shows various Lattice QCD determinations of HVP while the red results from hadronic decay of electron positron scattering (R-ratio),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

for Lattice QCD ensemble generation, Lattice QCD sampling for non-zero baryon density and sign problem, real-time lattice QCD formulation in Minkowski space-time, solving critical slowing down problem via trivializing maps, lattice QCD+QED and isospin breaking of hadrons and their decays, HLbL for $(g-2)_\mu$, nucleon electric dipole moment and matter-rich universe, nucleon anti-nucleon oscillation, proton decay, CP violating $K \to \pi\pi$ decay and ε'/ε, *etc.*

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

RBRC Researchers

Luchang JIN

Bollweg DENNIS

Special Postdoctoral Researcher

Nobuyuki MATSUMOTO

Visiting Scientists

Thomas BLUM (Univ. of Connecticut)
Hiroshi OKI (Nara Women's Univ.)
Akio TOMIYA (In'l Professional Univ. of Technology in Osaka)

List of Publications & Presentations

Publications

[Original Papers]

T. Blum, P. A. Boyle, M. Bruno, D. Giusti, V. Gülpers, R. C. Hill, T. Izubuchi, Y. C. Jang, L. Jin, and C. Jung *et al.,* arXiv:2301.08696.

T. Blum *et al.* [RBC and UKQCD], "Isospin 0 and 2 two-pion scattering at physical pion mass using all-to-all propagators with periodic boundary conditions in lattice QCD," Phys. Rev. D **107**, 094512 (2023).

J. S. Yoo, Y. Aoki, P. Boyle, T. Izubuchi, A. Soni, and S. Syritsyn, "Proton decay matrix elements on the lattice at physical pion mass," Phys. Rev. D **105**, 074501 (2022).

G. Rendon, T. Izubuchi and Y. Kikuchi, "Effects of cosine tapering window on quantum phase estimation," Phys. Rev. D **106**, 034503 (2022).

B. Chakraborty, M. Honda, T. Izubuchi, Y. Kikuchi, and A. Tomiya, "Classically emulated digital quantum simulation of the Schwinger model with a topological term via adiabatic state preparation," Phys. Rev. D **105**, 094503 (2022).

X. Gao, A. D. Hanlon, J. Holligan, N. Karthik, S. Mukherjee, P. Petreczky, S. Syritsyn, and Y. Zhao, "The Unpolarized Proton PDF at NNLO from Lattice QCD with Physical Quark Masses," arXiv:2212.12569.

X. Gao, A. D. Hanlon, N. Karthik, S. Mukherjee, P. Petreczky, P. Scior, S. Shi, S. Syritsyn, Y. Zhao, and K. Zhou, "Continuum-extrapolated NNLO valence PDF of the pion at the physical point," Phys. Rev. D **106**, 114510 (2022).

X. Gao, A. D. Hanlon, N. Karthik, S. Mukherjee, P. Petreczky, P. Scior, S. Syritsyn, and Y. Zhao, "Pion distribution amplitude at the physical point using the leading-twist expansion of the quasi-distribution-amplitude matrix element," Phys. Rev. D **106**, 074505 (2022).

X. Gao, A. D. Hanlon, S. Mukherjee, P. Petreczky, P. Scior, S. Syritsyn, and Y. Zhao, "Lattice QCD determination of the Bjorken-x dependence of parton distribution functions at next-to-next-to-leading order," Phys. Rev. Lett. **128**, 142003 (2022).

X. Gao, N. Karthik, S. Mukherjee, P. Petreczky, S. Syritsyn, and Y. Zhao, "Pion form factor and charge radius from Lattice QCD at physical point," Phys. Rev. D **104**, 11 (2021).

X. Gao, N. Karthik, S. Mukherjee, P. Petreczky, S. Syritsyn, and 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).

Y. Hamada and N. Matsumoto, "Energy of the boundary of spacetime," Prog. Theor. Exp. Phys. **2023**, 033B02 (2023).

N. Matsumoto, "Comment on the subtlety of defining a real-time path integral in lattice gauge theories," Prog. Theor. Exp. Phys. **2022**, 093B03 (2022).

X. Y. Tuo, X. Feng, and L. C. Jin, "Lattice QCD calculation of the light sterile neutrino contribution in $0\nu2\beta$ decay," Phys. Rev. D **106**, 074510 (2022).

Y. Fu, X. Feng, L. C. Jin, and C. F. Lu, "Lattice QCD calculation of the two-photon exchange contribution to the muonic-hydrogen lamb shift," Phys. Rev. Lett. **128**, 172002 (2022).

X. Feng, L. Jin, and M. J. Riberdy, "Lattice QCD calculation of the pion mass splitting," Phys. Rev. Lett. **128**, 052003 (2022).

X. Y. Tuo, X. Feng, L. C. Jin, and T. Wang, "Lattice QCD calculation of $K \to \ell\nu\ell\ell' + \ell'$-decay width," Phys. Rev. D **105**, 054518 (2022).

P. X. Ma, X. Feng, M. Gorchtein, L. C. Jin, and C. Y. Seng, "Lattice QCD calculation of the electroweak box diagrams for the kaon semileptonic decays," Phys. Rev. D **103**, 114503 (2021).

[Review Articles]

N. Craig, C. Csáki, A. X. El-Khadra, Z. Bern, R. Boughezal, S. Catterall, Z. Davoudi, A. de Gouvêa, P. Draper, and P. J. Fox *et al.*, "Snowmass Theory Frontier Report," arXiv:2211.05772.

Z. Davoudi, E. T. Neil, C. W. Bauer, T. Bhattacharya, T. Blum, P. Boyle, R. C. Brower, S. Catterall, N. H. Christ, and V. Cirigliano *et al.*, "Report of the snowmass 2021 topical group on lattice gauge theory," arXiv:2209.10758.

A. S. Kronfeld *et al.* [USQCD], "Lattice QCD and particle physics," arXiv:2207.07641.

P. Boyle, D. Bollweg, R. Brower, N. Christ, C. DeTar, R. Edwards, S. Gottlieb, T. Izubuchi, B. Joo, and F. Joswig *et al.* "Lattice QCD and the computational frontier," arXiv:2204.00039.

G. Colangelo, M. Davier, A. X. El-Khadra, M. Hoferichter, C. Lehner, L. Lellouch, T. Mibe, B. L. Roberts, T. Teubner, and H. Wittig *et al.* "Prospects for precise predictions of a_μ in the standard model," arXiv:2203.15810.

T. Blum, P. Boyle, M. Bruno, N. Christ, F. Erben, X. Feng, V. Guelpers, R. Hill, R. Hodgson, and D. Hoying *et al.*, "Discovering new physics in rare kaon decays," arXiv:2203.10998.

R. Alarcon, J. Alexander, V. Anastassopoulos, T. Aoki, R. Baartman, S. Baeßler, L. Bartoszek, D. H. Beck, F. Bedeschi, and R. Berger *et al.* "Electric dipole moments and the search for new physics," arXiv:2203.08103.

D. Bollweg, D. A. Clarke, J. Goswami, O. Kaczmarek, F. Karsch, S. Mukherjee, P. Petreczky, C. Schmidt, and S. Sharma, 'Equation of state and speed of sound of (2+1)-flavor QCD in strangeness-neutral matter at non-vanishing net baryon-number density," arXiv:2212.09043.

[Proceedings]

M. Engelhardt, N. Hasan, T. Izubuchi, C. Kallidonis, S. Krieg, S. Meinel, J. Negele, A. Pochinsky, G. Silvi, and S. Syritsyn, "Transverse momentum-dependent parton distributions for longitudinally polarized nucleons from domain wall fermion calculations at the physical pion mass," PoS **LATTICE2022**, 103 (2023).

P. Boyle, T. Izubuchi, L. Jin, C. Jung, C. Lehner, N. Matsumoto, and A. Tomiya, "Use of Schwinger-Dyson equation in constructing an approximate trivializing map," PoS **LATTICE2022**, 229 (2023).

J. S. Yoo, S. Syritsyn, Y. Aoki, P. Boyle, T. Izubuchi, and A. Soni, PoS **LATTICE2021**, 522 (2022).

J. S. Yoo, S. Syritsyn, Y. Aoki, P. Boyle, T. Izubuchi, and A. Soni, "Proton decay amplitudes with physical chirally-symmetric quarks on a lattice," PoS **PANIC2021**, 443 (2022).

M. Tomii, T. Blum, D. Hoying, T. Izubuchi, L. Jin, C. Jung, and A. Soni, "$K \to \pi\pi$ decay matrix elements at the physical point with periodic boundary conditions," PoS **LATTICE2021**, 394 (2022).

X. Feng, T. Izubuchi, L. Jin, and M. Golterman, "Pion electric polarizabilities from lattice QCD," PoS **LATTICE2021**, 362 (2022).

M. Engelhardt, J. Green, N. Hasan, T. Izubuchi, C. Kallidonis, S. Krieg, S. Liuti, S. Meinel, J. Negele, and A. Pochinsky *et al.,* PoS **LATTICE2021**, 413 (2022).

S. Foreman, T. Izubuchi, L. Jin, X. Y. Jin, J. C. Osborn, and A. Tomiya, "HMC with normalizing flows," PoS **LATTICE2021**, 073 (2022).

M. Fukuma, N. Matsumoto, and Y. Namekawa, "Applying the worldvolume hybrid Monte Carlo method to lattice field theories," PoS **LATTICE2022**, 011 (2023).

M. Fukuma, N. Matsumoto, and Y. Namekawa, "Numerical sign problem and the tempered Lefschetz thimble method," PoS **CORFU2021**, 254 (2022).

M. Fukuma and N. Matsumoto, "Tempered Lefschetz thimble method as a solution to the numerical sign problem," J. Phys. Conf. Ser. **2207**, 012054 (2022).

M. Fukuma and N. Matsumoto, "The basics and applications of the tempered Lefschetz thimble method for the numerical sign problem," PoS **LATTICE2021**, 395 (2022).

M. Fukuma, N. Matsumoto, and Y. Namekawa, "Worldvolume tempered Lefschetz thimble method and its error estimation," PoS **LATTICE2021**, 446 (2022).

P. A. Boyle, D. Bollweg, C. Kelly, and A. Yamaguchi, "Algorithms for domain wall Fermions," PoS **LATTICE2021**, 470 (2022).

Presentations

[International Conferences/Workshops]

S. Syritsyn (invited), "Nucleon electromagnetic form factors at large momentum from lattice QCD," Triangle Nuclear Theory Colloquium at UNC Chapel Hill, November 29, 2022.

S. Syritsyn (invited), "Nucleon electromagnetic form factors at large momentum from lattice QCD," Baryons 2022, Seville, Spain, November 7, 2022.

S. Syritsyn (invited), "Baryon number-violating amplitudes on a lattice with physical chirally-symmetric quarks," 14th Conference on the Intersections of Particle and Nuclear Physics (CIPANP), Orlando, FL, August 31, 2022.

S. Syritsyn (invited), "Nucleon & nuclear structure inputs to beyond-SM searches," SNOWMASS Rare Processes & Precision Frontier, Cincinnati, OH, May 17, 2022.

S. Syritsyn (invited), "Proton decay amplitudes with physical chirally-symmetric quarks," BNL-HET & RBRC Joint Workshop "DWQ@25," December 16, 2021.

S. Syritsyn (invited), "A more perfect universe: Role of lattice QCD in constraining violations of fundamental symmetries," Physics & Astronomy Colloquium, Stony Brook University, November 9, 2021.

L. Jin (Invited), "The hadronic light-by-light scattering contribution to the muon $g-2$," χ QCD annual collaboration meeting, Online, December 17, 2022.

L. Jin (Invited plenary talk), "Muon $g-2$ from lattice QCD," The 13th International Workshop on $e+e^-$ collisions from Phi to Psi, Online, August 17, 2022.

L. Jin (Invited), "Lattice QCD input for the first row CKM unitarity tests," Seattle Snowmass Summer Meeting 2022, Online, July 19, 2022.

L. Jin (Invited), "Combining infinite-volume photons and finite-volume hadronic matrix elements computed on the lattice," QED in Weak Decays, Higgs Centre for Theoretical Physics, JCMB, Online, June 24, 2022.

L. Jin (Invited), "The hadronic light-by-light scattering contribution to the muon $g-2$ (RBC/UKQCD)," SchwingerFest 2022: muon $g-2$, Physics and Astronomy Building, Mani L. Bhaumik Institute, UCLA, June 17, 2022.

L. Jin (Invited), "QCD + QED studies," USQCD All Hands' Meeting 2022, MIT, Online, April 22, 2022.

L. Jin (Invited), "Lattice calculation of the pion mass splitting using the infinite volume reconstruction method," χ QCD annual collaboration meeting, Online, December 19, 2021.

L. Jin, (Invited), "Attice calculation of the pion mass splitting using the infinite volume reconstruction method," BNL-HET & RBRC Joint Workshop "DWQ@25," Online, December 16, 2021.

L. Jin (Invited plenary talk), "Hadronic light-by-light contribution to muon $g-2$," The 10th International Workshop on Chiral Dynamics, Institute of High Energy Physics (IHEP), CAS, Online, November 19, 2021.

L. Jin (Invited), "Lattice calculation of the muon $g-2$," The first annual meeting of lattice QCD in China, Online, November 2, 2021.

L. Jin (Invited), "Lattice QCD input for the first row CKM unitarity tests," Fall Meeting of the Division of Nuclear Physics of the American Physics Society, DNP 2021, Online, October 13, 2021.

L. Jin (Invited), "Lattice QCD results on the hadronic contributions to the muon $g-2$," The XXVIII International Conference on Supersymmetry and Unification of Fundamental Interactions, SUSY 2021, Online, August 23, 2021.

L. Jin, "Pion electric polarizabilities from lattice QCD," LATTICE 2021, MIT, Online, July 29, 2021.

L. Jin (Invited), "Lattice calculation of the hadronic light-by-light contribution to the muon $g-2$ by the RBC-UKQCD collaborations," Muon $g-2$ theory initiative workshop in memoriam of Simon Eidelman, KEK IPNS, High energy physics laboratory in Nagoya University, Online, July 2, 2021.

L. Jin (Invited plenary talk), "Kaon decays from lattice QCD," Flavor Physics and CP violation (FPCP), Online, June 9, 2021.

L. Jin (Invited), "Quark and lepton flavor physics," DOE Virtual Annual Progress Review of USQCD, Online, May 18, 2021.

N. Matsumoto, "Search for an effective change of variable in QCD simulations," DWQ@25, USA (BNL), Online, December 13, 2021.

[Seminars]

N. Matsumoto, "Sign problem and worldvolume tempered Lefschetz thimble method, RIKEN Radiation Laboratory," Wako, Japan (RIKEN), Online, July 14, 2021.

N. Matsumoto, "Worldvolume tempered Lefschetz thimble method as an algorithm towards solving the sign problem," RBRC seminar, USA (BNL), Online, November 18, 2021.

N. Matsumoto, "Comment on the subtlety of defining real-time path integral in lattice gauge theories," Colorado University informal seminar, Colorado, USA, Online, July 21 2022.

N. Matsumoto, "Comment on the subtlety of defining real-time path integral in lattice gauge theories," KEK theory seminar, Tsukuba, Japan, Online, July 12, 2022.

N. Matsumoto, "Comment on the subtlety of defining real-time path integral in lattice gauge theories," Osaka University Particle Physics Group seminar, Osaka, Japan, Online, November 8, 2022.

N. Matsumoto, "Use of Schwinger-Dyson equation in constructing an approximate trivializing map," LATTICE 2022, Bonn, Germany, August 8, 2022.

L. Jin, "Lattice calculations in muon $g-2$," Department of Physics and Astronomy, University of California, Davis, Online, May 3, 2021.

L. Jin, "Lattice calculations in muon $g-2$," Hadron mass and structure forum, Online, April 20, 2021.

L. Jin, "Lattice calculations in muon $g-2$," Institute of Theoretical Physics, Chinese Academy of Sciences, Online, April 15, 2021.

L. Jin, "Muon $g-2$: hadronic light-by-light contribution and lattice QCD," Muon $g-2$ discussion forum, Peking University, Online, April 13, 2021.