Usage Report for Fiscal Year 2018

Project Title: Nucleon calculations for particle and nuclear physics

Name:

○Hiroshi Oki (1,2), Taku Izubuchi (1,3), Sergey Syritsyn (1,4), Chulwoo Jung(1,3), Yasumichi Aoki (1,5),

(1) RIKEN-BNL Research Center
(2) Nara Women's University
(3) Brookhaven National Laboratory, NY, USA
(4) Stony Brook University, NY, USA
(5) High Energy acceleration organization (KEK)

Laboratory at RIKEN:

RIKEN-BNL Research Center, Brookhaven National Laboratory

1. Background and purpose of the project, relationship of the project with other projects

Nucleons are basic building blocks of our visible universe, and understanding how quarks and gluons interacting via Quantum Chromodynamics (QCD) give rise to their rich structure is a central focus of both theory and experiment. Quarks can also participate in yet undiscovered interactions beyond the commonly accepted Standard Model (SM). High precision nuclear physics is a vital part of searches for new physics that can manifest itself in violation(s) of fundamental symmetries. In particular, observation of permanent electric dipole moments (EDMs) of nucleons and nuclei would be direct evidence for violation of CP symmetry. Connecting the quark- and hadron-level effective interactions is a task for QCD. It will also directly impact key measurements in the RHIC-Spin program and a future electron-ion collider (eRHIC), thus it is very important and timely calculation for RIKEN's experimental program at BNL.

Violation of this symmetry is required for baryogenesis, otherwise there would be no nuclear matter in the Universe. However, there is no presently known source of such violation at a required level, which is a strong promise for a discovery. The strong motivation for searches of CP violation is reflected in the long-range plan in its recommendation for a targeted program on fundamental symmetries, and it specifically emphasizes fundamental symmetry violations as the key question in understanding the origin of matter.

Using lattice QCD to calculate the structure of nucleons from first principles is one of the most important theoretic counterparts to these experimental efforts. Our precision calculations of hadron structure at the physical pion mass will for the first time enable predictions with broad physics impact. Approximately most of resources requested in our proposal have been used for computing electric dipole moments (EDMs) of protons and neutrons induced by effective quark-gluon interactions violating fundamental CP symmetry.

So far, most of lattice effort has been concentrated on nucleon EDMs induced by the θ-term, using either the background electric field method or $Q^2 \to 0$ extrapolation of the $F_3(Q^2)$ form factors, with results 1-2 orders of magnitude larger compared to QCD sum rules and chiral perturbation theory estimates. In the previous period of our project, <u>we have found that</u>

there is a problem in the conventional formula to extract the F_3 form factor commonly used in the previous lattice EDM calculations which use the nucleon-current correlation functions. In fact form factor calculations in previous literature suffered from unphysical contributions due to parity rotation of $e^{i\alpha_5\gamma_5}$ nucleon spinors not accounted for correctly, which lead to mixing of nucleon electric and magnetic moments and spurious contribution to the EDM. We show a comparison of two EDM results (F_3) between our correct formula and the conventional formula in Figure 1.

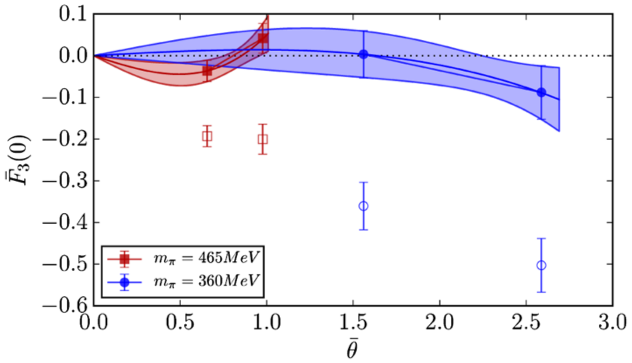

Figure 1: Corrected (filled symbols) and original (open symbols) values for the neutron form factors F_3 at a nonzero imaginary θ angle from Ref. [1].

Thus we have demonstrated that the previous EDM lattice computations which use the quark-current form factor receive a contribution from the spurious mixing effect by both theoretically and numerically computations of the CP-odd form factor and the energy shift using the CP violating cEDM operator. Our study for the correct treatment of the CP violating form factor in lattice QCD is one of our main achievements in our previous project, which was selected as one of editor's suggestions in the journal of Physical Review. (Ref. [2])

After appropriate corrections, all these previous results are compatible with zero within statistical error, and the "true" θ-induced nucleon EDM will be much harder to calculate. Therefore we have tested a recent technique of the truncation of space-time region of the topological charge to reduce the fluctuation of the EDM on lattice. Since this procedure introduces a systematic error, we also need to analyze the lattice data with a careful assessment of the truncation error. In this study, we use ensembles of QCD gauge configurations generated by the RBC/UKQCD collaboration employing Iwasaki gauge action and N_f =2+1 dynamical chiral-symmetric fermions with (Möbius) domain wall action (MDWF) (see Table 1). One ensemble has unphysical heavy pion mass m_π ≈ 340 MeV and is used to study the θ_{QCD}-induced nEDM. The most of the measurements of the θ_{QCD}-induced nEDM has been performed using GW-MPC at HOKUSAI.

$L_x^3 \times L_t \times L_5$	S_F[Ref]	m_π [MeV]	m_N [GeV]	Conf
$24^3 \times 64 \times 16$	DWF[3]	340(2)	1.178(10)	1400
$48^3 \times 96 \times 24$	MDWF[4]	139.2(4)	0.945(6)	130

Table 1: Gauge ensembles used in this study. The second column shows the action used and the reference where the ensemble was analyzed.

2. Specific usage status of the system and calculation method

The EDM is the forward limit of the P-,T-odd electric dipole form factor (EDFF) $F_3(Q^2)$

$$< N(p')|\bar{q}\gamma^\mu q|N(p) \geq \bar{u}\left[F_1(Q^2)\gamma^\mu + F_2(Q^2)\frac{i\sigma^{\mu\nu}q_\nu}{2M} - F_3(Q^2)\frac{\gamma_5\sigma^{\mu\nu}q_\nu}{2M}\right]u,$$

where q = p′ − p and $F_{1,2}$ are the regular parity-even Dirac and Pauli form factors. The EDM

$$d_n = \frac{e}{2M}F_3(0)$$

leads to P- and T- odd coupling of the nucleon spin and electromagnetic field with energy ΔE = $-d_N$ (S · E). Such an interaction can be induced by effective CP-violating interactions at the quark-gluon level represented by effective operators of increasing dimension and suppressed by the corresponding scale(s) of BSM physics. The only renormalizable (dimension=4) CP interaction is the QCD θ-term that may be present in the SM,

$$\mathcal{L} = \bar{\theta}\frac{1}{64\pi^2}\varepsilon^{\mu\nu\rho\sigma}G^a_{\mu\nu}G^a_{\rho\sigma},$$

where $\bar{\theta}$ is the anomaly-invariant combination of the QCD θ angle and quark mass phases. The most sensitive probes for the CP-violating interactions are electric dipole moment searches in hadronic, atomic, and molecular systems. In this proposal, we have measured nucleon 3- and 4-ponit correlation functions to determine the effect of quark chromo-electric dipole moments (cEDMs),

$$\mathcal{L}_{cEDM} = -i\sum_{q=u,d,s}\frac{\delta}{2}\bar{q}G^a_{\mu\nu}\varepsilon^{\mu\nu}\gamma_5 q,$$

and θ-induced nucleon EDMs, which can be detected from the P-, T-odd electric dipole form factor (F_3). Fortunately, our technique to compute nucleon form factors can be naturally extended to compute the CP-violating form factor F_3. A schematic algorithm for the 4pt function in terms of quark diagram is shown below using so-called (doubly) sequential source method for each of quark's vector current (dots) and cEDM interactions (crosses) (Figure 2).

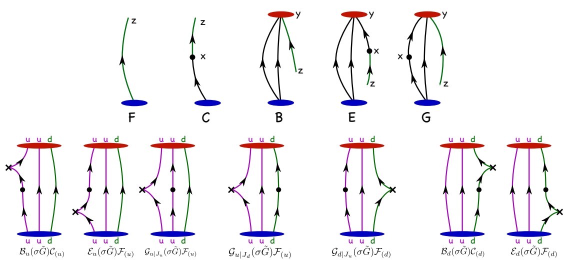

Figure 2: (Top) Sequential propagators required for computing four-point correlators and (Bottom) Fully-connected four-point correlation function for computing cEDM-induced nucleon electric dipole moment. Points indicate quark vector current and crosses show quark chromo-EDM operator insertions.

Studying θ_{QCD}-induced nEDM is complicated by the statistical noise due to the global nature of the topological charge. Its fluctuation $(\delta Q)^2 = \langle Q^2 \rangle \propto V_4$ grows with the lattice volume V_4 and leads to large statistical uncertainty in *CP*-odd correlation functions. As suggested in Refs. [5, 6], contributions to *Q* from distant sites may be neglected in computing nEDM. However, spatial restriction of *Q* may bias EDM results, for example if the "effective" parity mixing angle is different in the nucleon and the nucleon-current correlation functions. Such difference may be produced by non-identical spatial or timelike restriction of the partial topological charge in these *CP*-odd Green's functions, which results in nucleon interpolating operators acting on vacua with different amount of *CP* violation. To illustrate this point, consider the *CP* interaction that is turned on at some moment $t < 0$. The QCD vacuum takes some Euclidean time Δt to evolve into the new *CP*-violating vacuum state

$$|\text{vac}\rangle \rightarrow |\text{vac}\rangle_{CP}.$$

Nucleon operators acting on such transient vacuum state will have time-dependent overlap with the new nucleon-like states leading to ambiguity in the extracted values of the parity- mixing angle α5 and EDFF F_3. A similar argument applies to the nucleon sinks.

To avoid this ambiguity, in our study we restrict the topological charge estimator separately in time and space to a cylindrical volume V_Q (Figure 3),

$$\tilde{Q}(\Delta t_Q, r_Q) = \frac{1}{16\pi^2}\sum_{x\in V_Q}\text{Tr}\big[\hat{G}_{\mu\nu}\tilde{\hat{G}}_{\mu\nu}\big]_x\,,$$

$$(\vec{x},t)\in V_Q : \begin{cases} |\vec{x}-\vec{x}_0| \le r_Q\,, \\ t_0 - \Delta t_Q < t < t_0 + t_{\text{sep}} + \Delta t_Q\,, \end{cases} \qquad (1)$$

where t_0 is the location of the nucleon source and $t0 + t\text{sep}$ is the location of the nucleon sink. The *CP*-odd correlation functions are computed entirely inside the region defined in the above equation where *CP* violation is present (i.e. where the reduced topological charge $\tilde{Q}$ is sampled). The time-like cuts applied to $\tilde{Q}$ are symmetric with respect to the nucleon sources and sinks and equal in the nucleon and nucleon-current correlation functions. We should stress that the convergence with r_Q in Eq. (1) must be verified at each nucleon momenta to avoid bias, especially in computing the Q_2-dependence of the EDFFs.

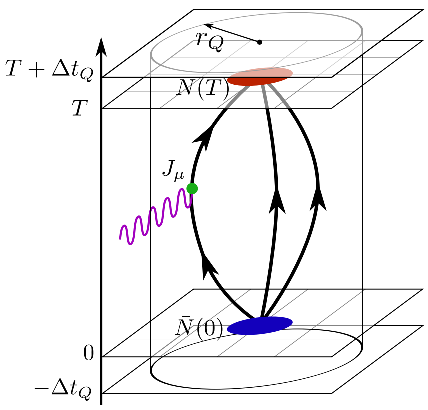

Figure 3: Constrained sampling of the topological charge density (1) for reducing the statistical noise in the *CP*-odd three-point correlation functions, as well as the *CP*-odd two-point correlation functions.

3. Result

We study the effect of reduced topological charge sampling on the mixing angle α_5. The mixing angle α_5 is estimated with the $\{t,\Delta t_Q,r_Q\}$-dependent ratio of the nucleon two-point functions with and without insertion of CP-violating source at $m_\pi \approx 340$ MeV. Results for different values of t_Q,r_Q are shown in Figure 4. It is found that the convergence to the result obtained with the full topological charge Q (r_Q, $\Delta t_Q \rightarrow \infty$) for $\Delta t_Q > 8a$, where a is a lattice spacing). However, for the spatial cut r_Q there is no convergence up to $r_Q \approx 12a$, which is $\approx 52\%$ of the spatial volume. We conclude that the lattice volume $V^3 = (24a)^3 \approx (2.7\ \mathrm{fm})^3$ is insufficient to benefit from the spatial cut r_Q, and should be explored with larger spatial volumes. The neutron and proton electric dipole form factors computed for a range of Δt_Q, r_Q values are shown in Figure 5, where only the connected diagrams are computed. We observe statistically significant value for the neutron F_3 even with the full value of the topological charge Q, which has no bias from reduced

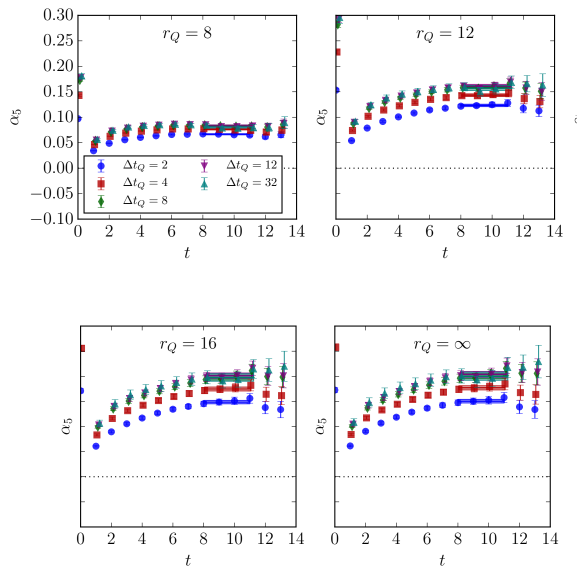

Figure 4: The nucleon parity mixing angle and its dependence on the spatial and temporal cuts in the reduced topological charge at $m_\pi \approx 340$ MeV.

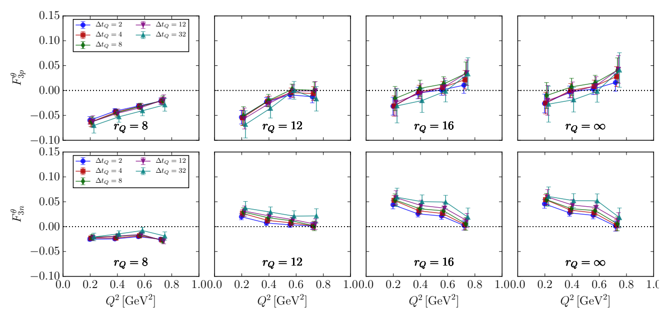

Figure 5: Proton and neutron electric dipole form factors induced by the θ_{QCD}-term from lattice calculations with $m_\pi \approx 340$ MeV (only connected contractions) and their dependence on the spatial and temporal cuts in the reduced topological charge ($\Delta t_Q,r_Q$).

sampling. We can make a very preliminary estimate for the value of the F_3 form factor which should only be used to check the consistency with the phenomenology and earlier lattice QCD results, since this results has almost 100% error due excited state contaminations and the uncertainty of the zero momentum extrapolation. Actually our result at heavier π mass is consistent with the value obtained using Wilson fermion [1], which gives a constraint $|F^{\theta}_3(Q^2=0)| < 0.06$.

Using our rough estimate for F^{θ}_3, we can project the effort required for computing nEDM at the physical point. We performed initial calculations using ensembles at physical quark mass with larger volume with ~33,000 statistics (See Table 1). We observe no signal for the neutron EDFFs (See Figure 6), and the results are consistent with zero with the statistical uncertainty.

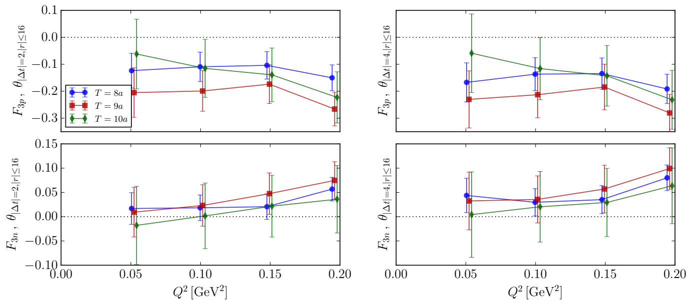

Figure 6: Proton and neutron electric dipole form factors induced by the θ_{QCD}-term from lattice calculations with physical quark masses.

4. Conclusion

Calculations of nEDM on a lattice are important for interpreting constraints or results from nucleon and nuclei EDM measurements. Calculations of θ_{QCD} induced nEDM with a truncated topological charge method has been tested. It is found that the convergence to the result for the mixing angle obtained with the full topological charge. We observe statistically significant value for the neutron F_3 even with the full value of the topological charge Q, which has no bias from reduced sampling. However, for the spatial cut r_Q there is no convergence and our method should be explored with larger spatial volumes.

5. Schedule and prospect for the future

θ_{QCD}-induced EDM at the physical point will be challenging and will require special techniques to tame the statistical noise caused by fluctuations of the global topological charge. Direct calculations at the physical point may be at the limit of the current computing capabilities since our preliminary result shown in sec. 3 indicates that the expected signal-to-noise ratio ~ 0.2 at physical point has to be improved by a factor of 5-10 which requires × (25~100) more statistics to obtain the non-zero signal for EDFF. In order to improve the statistical accuracy, we would like to employ alternative computing methods such as dynamical (imaginary) θ^I term. We plan to generate a QCD gauge ensemble with an RHMC algorithm using a QCD action with additional CP-violating gauge action. Since the computations of the nucleon EDM depend on contributions from non-trivial topological sectors, dynamical θ^I-term becomes more important at lighter quark masses, where the light quarks suppress the topological fluctuations.

References

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Usage Report for Fiscal Year 2018

Fiscal Year 2018 List of Publications Resulting from the Use of the supercomputer

[Conference Proceedings]

[1] Sergey Syritsyn, Taku Izubuchi, and Hiroshi Ohki, “Progress in the Nucleon Electric Dipole Moment Calculations in Lattice QCD” , proceedings of CIPANP2018 - Thirteenth Conference on Intersections of Particle and Nuclear Physics, Palm Springs, CA, USA, May 29- June 3, 2018.

[2] Sergey Syritsyn, Taku Izubuchi, and Hiroshi Ohki, “Calculation of Nucleon Electric Dipole Moments Induced by Quark Chromo-Electric Dipole Moments and the QCD θ-term” , proceedings of XIII Quark Confinement and the Hadron Spectrum – Confinement 2018, Maynooth University, Ireland, July 31 – August 6, 2018.

[Oral presentation]

[3] Sergey Syritsyn, "Progress on the Nucleon EEDM in lattice QCD", presentation at CIPANP2018 - Thirteenth Conference on Intersections of Particle and Nuclear Physics, Palm Springs, CA, USA, May 29, 2018.

[4] (**Invited talk**) Sergey Syritsyn, "Progress on the Nucleon EDM in Lattice QCD", presentation at XIII Quark Confinement and the Hadron Spectrum – Confinement 2018, Maynooth University, Ireland, August 1.

[3] Taku Izubuchi, "Nucleon Form factor calculation using DWQCD", presentation at the 36th Annual International Syposium on Lattice Field Theory (Lattice2018), Michigan, USA, July 27, 2018.

[4] (**Invited talk**) Hiroshi Oki, Nucleon Electric Dipole Moments from Lattice QCD, 基研研究会 素粒子物理学の進展 2018, August 6 – 10, Kyoto University, Kyoto.