

## Dynamical QCD simulation with $\theta$ terms

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The  $\theta$  term that breaks the Strong CP symmetry is introduced in the two flavors of dynamical QCD simulation.  $\theta$  is analytically continued to a pure imaginary number to make the probability of Monte Carlo positive. The Neutron's Electric Dipole Moment (NEDM) is measured on the ensemble under a uniform and weak electric field. Other applications of  $\theta$  terms are also discussed.

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## 1. Introductions

Since the first attempt to get the non-perturbative prediction of the Neutron's Electric Dipole Moment (NEDM) with the Strong CP violating  $\theta$  term,

$$S_\theta = i \frac{\theta}{32\pi^2} \int \varepsilon_{\mu\nu\tau\rho} F_{\mu\nu} F_{\tau\rho} d^4x = i\theta Q_{\text{top}} , \quad (1.1)$$

on lattice 18 years ago [1], there have been renewed interests on this calculation recently corresponding to the new experiments and theoretical developments. The NEDM is very sensitive to the sea quark mass, as we will see, and the calculation could be much improved thanks to the recent various developments for the simulation with dynamical quarks.

All the calculations aiming for NEDM so far introduce the effect of  $S_\theta$  in terms of reweighting technique: the statistical ensembles of QCD vacuum were generated via the Boltzmann weight of  $\theta = 0$  case,  $\text{Prob}(U) \propto \det^{N_f} D[U] e^{-S_0[U]}$ , and then the effect of  $S_\theta$  is treated as a part of observable in the measurement stage,  $\langle \mathcal{O} \rangle_\theta = \sum_U \mathcal{O} e^{-S_\theta} \text{Prob}(U) / \sum_U 1 e^{-S_\theta} \text{Prob}(U)$ .

In this study, we introduce the CP violation according to  $S_\theta$  in the probability of QCD ensemble generation, then measure observables without reweighting technique to see whether the new way of calculation has better control over the statistical and the systematic errors. To keep the Boltzmann weight positive semi definite, the value of  $\theta$  is analytically continued to pure imaginary,

$$\theta \rightarrow -i\theta. \quad (1.2)$$

Such analytic continuation was previously explored for  $\text{CP}^{n-1}$  models with  $\theta$  term [2] and QCD with the chemical potential [3].

To measure NEDM, a constant electric field,  $\vec{E}$ , is applied to Nucleon, and the energy,  $m_N$ , dependence on its spin polarization,  $\vec{S}$ , is measured,

$$m_N(\vec{E}, \vec{S}) - m_N(\vec{E}, -\vec{S}) = 2id_N(\theta) \vec{S} \cdot \vec{E} + \mathcal{O}(E^3) . \quad (1.3)$$

We use electric field constituted from the ordinary U(1) gauge field,

$$U_\mu^{\text{EM}}(x) = e^{iqA_\mu^{\text{EM}}(x)}, \quad qA_\mu^{\text{EM}}(x) \in \mathbb{R} , \quad (1.4)$$

on *Euclidean* lattice, oppose to its *Minkowski* space version used in the original calculation [1], which is reported to be susceptible to the systematic error induced at the periodic boundary in temporal direction [4]. To avoid the boundary effect and also to safely neglect the  $\mathcal{O}(E^3)$  in (1.3) at a time, a *uniform and weak electric field* invented some times ago [5, 6] is implemented.

By assuming  $\theta$  is small, the NEDM,  $d_N(\theta)$ , is expanded in terms of  $\theta$ ,

$$d_N(\theta) = d_N^{(1)} \theta + \mathcal{O}(\theta^3) , \quad (1.5)$$

within which approximation, the analytic continuation, (1.2), can be trivially reverted, and more importantly, the energy splitting (1.3) becomes a real number, which could be easily measured from the ratio between polarized propagators of Neutron whose spin are parallel and anti-parallel to the direction of the electric field,

$$R(t, t_{\text{src}}; E) = \lim_{t \rightarrow \text{large}} \frac{\langle N_\uparrow(t) \overline{N}_\uparrow(t_{\text{src}}) \rangle_{\theta, E}}{\langle N_\downarrow(t) \overline{N}_\downarrow(t_{\text{src}}) \rangle_{\theta, E}} \propto e^{-d_N \theta E t} . \quad (1.6)$$

In the following sections, the NEDM calculation and preliminary results are mainly detailed. We also briefly report another related attempt, restricting the imaginary  $\theta$  action to a time slice and identifying it as the source term for the flavor-singlet pseudoscalar meson ( $\eta'$ ) for disconnected quark loop measurements.

## 2. Ingredients for NEDM

Before describing the novel simulation setups, we compare the external electric field method employed in this work with another method, the form factor calculation [7, 8], in which NEDM is calculated from the CP-odd form factor,  $F_3(q^2)$ . While the latter method is free from the  $\mathcal{O}(E^3)$  contamination in (1.3), one needs to inject momentum  $q$  to the vector current of the Nucleon's three point function, and extrapolate  $q^2 \rightarrow 0$  limit. We chose the simpler method, the external electric field method, that involves only two point functions with zero momentum, expecting the statistical and/or systematic error could be smaller than the other.

### 2.1 Dynamical simulation with $\theta$ terms

All the previous lattice QCD calculations with the strong CP breaking term  $S_\theta$ , (1.1), were carried out with the reweighting technique as discussed in Sec. 1. Alternatively, one could put  $S_\theta$  into the ensemble probability if  $S_\theta$  becomes real number by  $\theta$  being analytically continued to pure imaginary, (1.2). There are two options in the implementation of  $S_\theta$  on lattice: one is the gluonic definition from  $\sum_x F\tilde{F}(x)$  with an appropriate smeared/cooled link field so that the resulting topological charge,  $Q_{\text{top}}$ , become (close to) an integer value. This implantation may be useful for a certain application such as precise determination of the  $Q_{\text{top}}$  distribution in pure Yang-Mills theory [9]. Actual simulation coding, however, might likely involve the smeared/cooled gauge force term, and results could strongly depend on the details of the smearing/cooling used. Simpler implementation would be using the anomalous axial transformation in the continuum theory,

$$\psi \rightarrow e^{-i\theta\gamma_5/(2N_f)}\psi, \quad \bar{\psi} \rightarrow \bar{\psi}e^{-i\theta\gamma_5/(2N_f)} \quad (2.1)$$

$$\mathcal{D}\psi\mathcal{D}\bar{\psi} \rightarrow \mathcal{D}\psi\mathcal{D}\bar{\psi} e^{S_\theta}, \quad (2.2)$$

that cancels the  $S_\theta$  from the original action at the cost of CP violating  $\gamma_5$  mass term introduced in the fermion's Lagrangian for  $N_F = 2$ ,

$$\mathcal{L}_f = \sum_{i=u,d} \bar{\psi}_i (\mathcal{D} + m + im\frac{\theta}{2}\gamma_5)\psi_i + \mathcal{O}(\theta^2). \quad (2.3)$$

We chose the latter implementation because of the absence the ambiguity from cooling/smearing. By the analytic continuation, (1.2), the fermion determinant with the  $\gamma_5$  mass term in (2.3) remains positive:  $\det(\mathcal{D} + m + im\frac{\theta}{2}\gamma_5)^2 \rightarrow |\det(\mathcal{D} + m + m\frac{\theta}{2}\gamma_5)|^2$ .

Our lattice fermion action is the RG improved clover fermion identifying the continuum counter parts as follows:

$$\mathcal{D} + m \rightarrow D^{\text{clover}}, \quad im\frac{\theta}{2}\gamma_5 \rightarrow i(m - m^c)\frac{\theta}{2}\gamma_5, \quad (2.4)$$

where  $m^c$  is the mass point where the pseudoscalar meson becomes massless.

We note the relation, (2.2) (2.3), are not be precisely realized for the clover fermion and there will be a discretization error which will vanish in the continuum limit. More demanding simulation with overlap fermion or domain-wall fermions might be free from such systematic error.

## 2.2 Uniform and weak electric field

The second ingredients for NEDM is the external electric field on the periodic lattice. The electric field needs to be weak and constant everywhere including the periodic boundaries as discussed in Sec. 1. Naively discretize the constant electric field in the continuum theory, for example, in  $z$  direction,  $A_z^{\text{EM}}(x) = Et$  in terms of vector potential, one obtains  $U_z^{\text{EM}} = \exp(iqEt)$  for charge  $q$  fermion field. This Abelian link field gives constant electric field,  $e^{iF_t z} = e^{iqE}$ , everywhere except at the boundary between  $t = L_t - 1$  and  $t = 0$ , where the strong opposite electric field,  $\exp(-iqE(L_t - 1))$ , is induced. This delta function like field causes a skewed Neutron propagator near the boundary [4]. By using the constructions in [5, 6], such systematic error could be avoided by adjusting the temporal link, only at the boundary, as

$$U_t^{\text{EM}}(z, L_t - 1) = \exp(-iqE(L_t - 1)z) , \quad E = \frac{q2\pi}{L_t L_z} \times \mathbb{Z} , \quad (2.5)$$

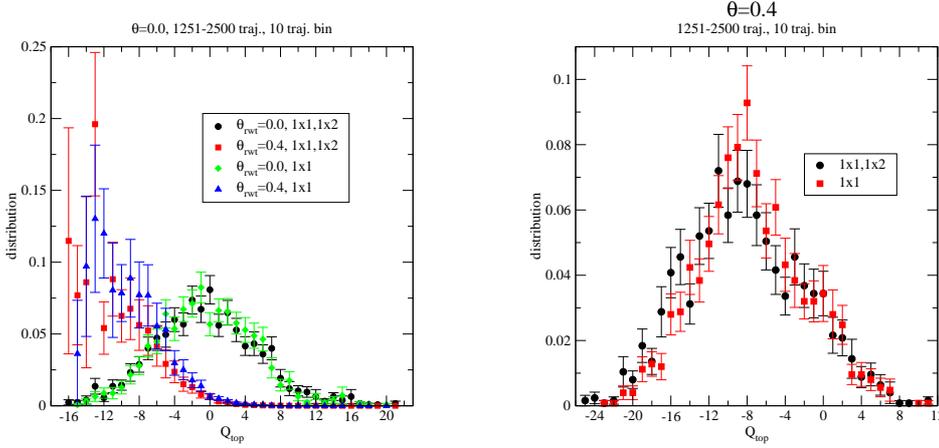
where the condition (2.5) is required not to induce another opposite field at the corner plaquette, including points  $(z, t) = (L_z - 1, L_t - 1)$  and  $(0, 0)$ , of the periodic boundaries. We emphases this construction has weaker electric field,  $E \sim 0.01q \times \mathbb{Z}$  than the simpler construction with  $E = 2\pi/L_t$  so that  $\mathcal{O}(E^3)$  contamination in (1.3) is less problematic.

## 3. Progress report on NEDM calculation

We now report the preliminary results of NEDM calculation with the setups described in Sec. 2 employed on  $16^3 \times 32$  lattice. The gauge action of our choice is the RG improved gauge action a la Iwasaki with  $\beta = 2.1(a^{-1} \sim 2\text{GeV})$ . Thermalized statistical ensembles of two flavors of dynamical clover fermion action ( $c_{\text{sw}} = 1.47$ ) with  $\theta = 0.4$  and  $0.0$  are accumulated for  $\tau = 2,000$  in the molecular dynamics time unit. The parameter point are taken from tadpole .... by CP-PACS [?]. The effect of  $\theta$  vanishes at massless limit as seen in (2.3). As this is a feasibility study, we consciously set the quark mass unphysically large,  $\kappa = 0.1357$  or  $m_\rho/m_\pi \sim 0.85$ . The HMC code with accelerations a la Sexton-Weingarten, and also Hasenbush is used.

By switching on  $e^{-S_\theta} = e^{-\theta Q_{\text{top}}}$  in the Boltzmann weight, the negative topological charge should appears more frequently than the positive charge for  $\theta > 0$ . Figure 1 clearly shows such reaction to  $\theta$ . The positive and negative charge are equally appears for  $\theta = 0$  in the Gaussian-like distribution, which is shifted in negative direction,  $\langle Q \rangle = -7.9$ , for  $\theta = 0.4$  ensemble. Here we plot the distribution of the  $\mathcal{O}(a^2)$  improved topological charge defined from the gluon configuration,  $Q_{\text{top}} = \frac{5}{3}Q^{1 \times 1} - \frac{2}{3}Q^{2 \times 1}$ , where  $Q^{1 \times 1}$  and  $Q^{1 \times 2}$  are topological charges calculated from  $1 \times 1$  and  $1 \times 2$  clover leafs respectively [10]. The lattice are smoothed until  $Q_{\text{top}}$  becomes saturated close to an integer value. Applying 200 steps of APE smearing ( $c_{\text{APE}} = 0.45$ ) turns out to be needed.

The polarized Neutron propagator is measured using the code developed in [?] on 100 configurations under the external electric field, that is a multiple of,  $E_0 = 2\pi/(L_z L_t) \times 3 \simeq 0.0368$ , in  $z$  direction. The quark charges are set as  $q_{\text{up}} = 2/3$  and  $q_{\text{down}} = -1/3$ . On each lattice, two sources



**Figure 1:** The distributions of  $Q_{\text{top}}$  for  $\theta = 0.0$  (left) and  $\theta = 0.4$  (right).  $Q_{\text{top}}$  is calculated by  $\mathcal{O}(a^2)$  improved definition on 200 steps of APE smeared ( $c_{\text{APE}} = 0.45$ ) lattices. Also the definition only uses  $1 \times 1$  plaquette is plotted. The distribution for  $\theta = 0.4$  by the reweighting technique is plotted on the left figure to show the poor predictability for such sizable  $\theta$ .

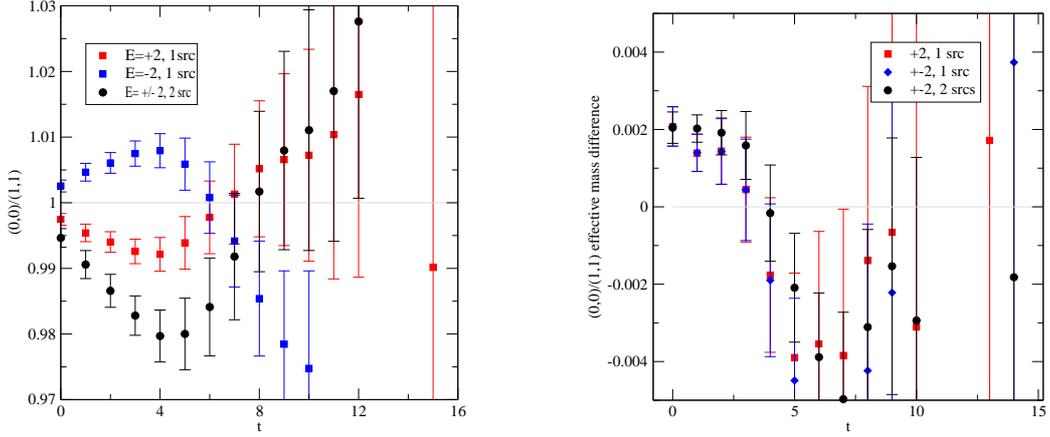
for Neutron made of the Gaussian smeared quarks are prepared, and the propagators of Nucleon are measured for each sources separately.

The spin dependent ratio of the propagator, (1.6), is estimated from the propagator averaged with the one with the other source points, and also with the one applied the opposite electric field with the appropriate combination as follows:

$$R_2(t - t_{\text{src}}) = \prod_{t_{\text{src}}} \left( \frac{R(t, t_{\text{src}}; E)}{R(t, t_{\text{src}}; -E)} \right)^{1/(2N_{\text{src}})}. \quad (3.1)$$

Thanks to the temporal translational invariance of the external electric field described in Sub-Sec. 2.2, the backward propagator of the anti-Neutron at  $t - t_{\text{src}} < 0$  may also be used in the average to enhance the signal. While a reasonable signal for  $t - t_{\text{src}} \lesssim 4$  can be seen within current statistics, we need more ensemble and measurements to check the excited state contamination. We also compare  $R_2(t)$  using the traditional reweighted technique on  $\theta = 0$  lattice with same statistics, and found about a factor of two smaller statistical error for the new method.

Due to lack of the chiral symmetry in clover fermion action and also from  $\mathcal{O}(\theta^2)$  in (2.3),  $\theta$  in (2.3) may be mixed with different operators. To check the effect of  $\theta$  in other quantities than NEDM, we calculate the shift of topological charge  $\langle Q_{\text{top}} \rangle_{\theta}$  and pseudoscalar meson mass  $M_{PS}(\theta)$  on  $\theta = 0.4$  configuration. For crude estimates of effective  $\theta$  value on this ensemble, we assume Gaussian distribution for  $Q_{\text{top}}$ , and the leading order prediction of chiral perturbation theory,  $M_{PS}^2(\theta) = M_{PS}^2(0) \cosh(\theta/N_f)$  in [11]. The ratio of the effective  $\theta$ s obtained by these method to the input value, 0.4, turn out to be 0.6(1) from  $\langle Q_{\text{top}} \rangle_{\theta}$ , and 0.9(5) from pseudoscalar mass.



**Figure 2:** The double ratio,  $R_2(t - t_{src}) = \prod_{t_{src}} (0,0)/(1,1)$  (left), and its effective mass  $\log(R(t)/R(t+1))$  (right) are plotted. The applied external electric fields are  $E = +2E_0$  (red),  $E = -2E_0$  (blue), and the appropriate average over  $E = \pm 2E_0$  (black). The red and green symbols are calculated using one source points while the block symbols is the average of two source results.

#### 4. Application for $\eta'$ calculation

If we generate ensemble replacing  $S_\theta$  by

$$S_\lambda = \lambda \sum_{\vec{x}} \bar{\psi} \gamma_5 \psi(\vec{x}, t_s) , \quad (4.1)$$

which is the source term enhancing the negative topological charge density only at a time slice  $t = t_s$ , the resulting configurations could be used to measure quantities involve the disconnected quark loop. Here we present a calculation of the flavor-singlet pseudoscalar meson ( $\eta'$ ) propagator as an example.

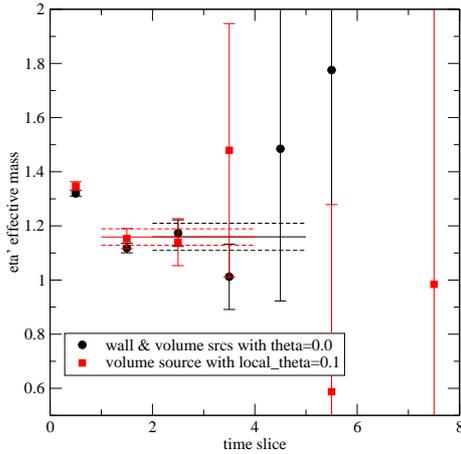
The pseudoscalar density at  $t$  with the Dirac operator including the  $\lambda$  term,  $D_\lambda$  is estimated stochastically,

$$\langle \text{Tr} \gamma_5 D_\lambda^{-1}(t, t) \rangle_\lambda = -\lambda \langle \text{Tr} \gamma_5 D^{-1}(t, t_s) \gamma_5 D^{-1}(t_s, t) \rangle_0 + 2\lambda \langle \text{Tr} \gamma_5 D^{-1}(t, t) \text{Tr} \gamma_5 D^{-1}(t_s, t_s) \rangle_0 + \mathcal{O}(\lambda^3) , \quad (4.2)$$

whose left hand side is the  $\eta'$  correlation function between  $t_s$  and  $t$  omitting  $\mathcal{O}(\lambda^3)$ . The result of effective mass on 1,000 configuration of  $8^3 \times 16, a \sim 0.2\text{fm}$  lattice is shown in Figure 3 compared with the conventional two point function method (black circle). The central value is consistent with each other, however, the source method has much rapid error growth by increasing  $t - t_s$ .

#### 5. Summary and Conclusion

We have generated  $N_F = 2$  lattice QCD ensemble with the explicit CP violation term,  $\theta$  term. To preserve the positivity of the generating probability,  $\theta$  is analytically continued to pure imaginary. By applying the uniform and weak electric field on the ensemble, Nucleon's electric dipole moment is calculated. While the results are only on two parameter points, the signal to noise ratio



**Figure 3:** The effective mass of the flavor singlet pseudoscalar meson as a function of time using the source method compared with the conventional two point function method.

observed is encouraging considering the relatively small statistics. The checks for the excited state contamination by increasing statistics, effects of the higher order term effect in  $\theta$  and  $E$ , and the quark mass dependence are subjects for future study.

We also explore QCD ensemble with the source for the flavor singlet pseudoscalar density. The propagator of the flavor singlet pseudoscalar meson,  $\eta'$ , is calculated by restricting the imaginary  $\theta$  term on a time slice, consistent results with the conventional method are obtained though the statistical error turns out to be larger than that from the conventional method.

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