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η' meson mass from topological charge density correlator in QCD

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The flavor-singlet component of the η' meson is related to the topological structure of the SU(3) gauge field through the chiral anomaly. We perform a $2 + 1$ -flavor lattice QCD calculation and demonstrate that the two-point function of a gluonically defined topological charge density after a short Yang-Mills gradient flow contains the propagation of the η' meson, by showing that its mass in the chiral and continuum limit is consistent with the experimental value. The gluonic correlator does not suffer from the contamination of the pion contribution, and the clean signal is obtained at significantly lower numerical cost compared to the conventional method with the quark bilinear operators.

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Among other hadrons the η' meson plays a special role in the study of the topological structure of QCD. The η' meson would be a pseudo-Nambu-Goldstone boson associated with the spontaneous breaking of the axial $U(1)$ symmetry, while it acquires a large mass through the chiral anomaly [1], which relates the divergence of the flavor-singlet axial vector current to the topological charge density in QCD. Witten [2] and Veneziano [3] estimated the η' meson mass in the large- N_c (number of colors) limit and showed that its mass squared is proportional to the topological susceptibility of QCD.

In real QCD with $N_c = 3$ and light dynamical quarks, the argument of Witten and Veneziano is no longer valid. It is not the η' meson but the pion that governs the topological susceptibility. In fact, in our previous lattice QCD simulations where we kept the chiral symmetry (nearly) exact [4–6], it was confirmed that the topological susceptibility is proportional to the light sea quark masses as predicted by chiral perturbation theory, $\chi_t = \frac{\Sigma}{\sum_i 1/m_i}$, where Σ denotes the chiral condensate and m_i denotes the i th light quark mass. In particular, χ_t vanishes in the limit of massless up and down quarks, reflecting the long-range dynamics of the pion field.

Then, an interesting question arises: what happens to the η' meson with $N_c = 3$? Since the effect of the anomaly is stronger than in the large- N_c limit, the η' meson mass should be still generated by the topological fluctuation of the gluons. Nevertheless, it must be insensitive to χ_t . This implies a nontrivial double-scale structure in the topological excitation of gauge field: it creates the η' meson at short distances, while making a tight connection to the pion at long distances. The answer to this question could be that

the topological property of the η' meson in QCD is hidden inside the pion clouds.

In this work, by an explicit calculation in $2 + 1$ -flavor lattice QCD, we show that the two-point function of the topological charge density at short distances gives a mass consistent with the experimental value of the η' meson mass. Since we have computed χ_t using the same correlation functions (see Ref. [6] for the details), our data clearly show the double-scale structure of the topological property of gluons: the long-range physics described by the pion and the short-range (or first excited) physics governed by the η' meson.

Not only is it theoretically interesting, but our work also proposes a practically advantageous method to determine the η' meson mass. Direct lattice calculation of the η' meson mass has been challenging because one has to include the disconnected quark-line diagram, which appears from the Wick contraction of the fermion bilinear operators representing the $J^{PC} = 0^{-+}$ flavor-singlet state, as has been done in recent calculations [7–11]. This is numerically demanding and statistically very noisy.

The advantage of the gluonic calculation adopted in this work over the conventional fermionic one is twofold. First, we can avoid the enormous computational cost of stochastically evaluating the disconnected diagram. The gluonic definition of the topological charge density does not require any inversion of the Dirac operator.

Second, our method avoids the contamination from the pions. In the conventional method where one calculates quark connected and disconnected diagram contributions appearing from the Wick contraction of quark fields, the pion may propagate in each contribution, but it cancels between them. A large statistics is required for a sufficient

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cancellation before extracting the η' meson propagator. Since the purely gluonic definition of the topological charge density operator

$$q(x) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \text{Tr} F_{\text{cl}}^{\mu\nu} F_{\text{cl}}^{\rho\sigma}(x), \quad (1)$$

where $F_{\text{cl}}^{\mu\nu}$ denotes the field strength tensor of the gluon field defined through the so-called clover term consisting of four plaquettes, does not directly couple to the pions, its correlator is free from the pion background.

Note here that the sum of (1) over the lattice volume gives the global topological charge up to discretization effects, $Q = \sum_x q(x) + \mathcal{O}(a^2)$. However, it is well known that the $\mathcal{O}(a^2)$ contribution is large with currently available lattice spacings. In order to reduce this statistical noise, we modify the link variables using the Yang-Mills (YM) gradient flow [12]. At a flow time t , it amounts to smearing the gauge fields in a range of the length $\sqrt{8t}$. It is shown that the topological charge Q defined through (1) converges to an integer value at a sufficiently large flow time [13,14]. This smearing procedure eliminates short-distance fluctuations and also suppresses the noise at longer distances.¹

For our purpose of extracting the η' meson mass, the YM gradient flow time has to be short in order not to distort the correlation of the η' propagation. Assuming a simple Gaussian form of the smearing effect, Bruno *et al.* [20] estimated the size of distortion of the correlator as

$$\frac{\Delta\langle q(x)q(y) \rangle}{\langle q(x)q(y) \rangle} \sim e^{-(|x-y|/\sqrt{8t}-m_{\eta'}\sqrt{8t})^2} \frac{m_{\eta'}(8t)^{3/2}}{2\sqrt{\pi}|x-y|^2}. \quad (2)$$

In our analysis below, we use the reference flow time around $\sqrt{8t} = 0.2$ fm for the fit range $|x-y| > 0.6$ fm, which makes the above correction less than 1% for $m_{\eta'} \simeq 1$ GeV.

We employ the Symanzik gauge action and the Möbius domain-wall fermion action for gauge ensemble generations [21–23]. We apply three steps of stout smearing of the gauge links before inserting it in the Dirac operator. Our main runs of $2+1$ -flavor lattice QCD simulations are carried out on two different lattice volumes $L^3 \times T = 32^3 \times 64$ and $48^3 \times 96$, for which we set $\beta = 4.17$ and 4.35, respectively. The inverse lattice spacing $1/a$ is estimated to be 2.4 GeV (for $\beta = 4.17$) and 3.6 GeV (for $\beta = 4.35$), using the input $\sqrt{t_0} = 0.1465$ fm [24] where the reference YM gradient flow time t_0 is defined by $t^2\langle E \rangle|_{t=t_0} = 0.3$ [12], with the energy density E of the gluon field. Our two lattices share a similar physical size $L \sim 2.6$ fm. For the quark mass, we use two values of the

strange quark mass m_s around its physical point and three to four values of the up and down quark mass m_{ud} for each m_s . The lightest pion mass is around 230 MeV with our smallest value of $am_{ud} = 0.0035$ at $\beta = 4.17$. In order to check the systematics due to finite volume sizes and lattice spacings, we also perform simulations on a larger lattice $48^3 \times 96$ (at $\beta = 4.17$ and $m_\pi \sim 230$ MeV) and a finer lattice $64^3 \times 128$ (at $\beta = 4.47$ [$1/a \sim 4.5$ GeV] and $m_\pi \sim 285$ MeV). For each ensemble, 500–1,000 gauge configurations are sampled from 10,000 molecular dynamics (MD) time. The residual mass in the Möbius domain-wall fermion formalism is kept smaller than ~ 0.5 MeV [25] by choosing $L_s = 12$ at $\beta = 4.17$ and $L_s = 8$ at $\beta = 4.35$ (and 4.47).

On each generated configuration, we perform 500–1,000 steps of the YM gradient flow (using the conventional Wilson gauge action) with a step size $a^2\Delta t = 0.01$. At every 20–30 steps, we store $q(x)$ and measure its correlator using the fast Fourier transform (FFT) technique. As reported in Ref. [6], the flow time history of the gluonic definition of the topological charge Q shows a good convergence to discrete values near integers.

We find that the two-point function $\langle q(x)q(y) \rangle$ at our target distance $|x-y| \sim 0.7$ fm always shows a shorter autocorrelation time than 10 MD time, while its global average, $Q = \sum_x q(x)$, has $\mathcal{O}(100)$ or higher MD time at $\beta = 4.35$. This is a good evidence that the η' meson physics is *decoupled* [26] from the global topological charge. In the following analysis, we estimate the statistical error by the jackknife method after binning the data in 140–200 MD time.

Figure 1 shows the topological charge density correlator $C(|x-y|) = -\langle q(x)q(y) \rangle$ at the flow times $a^2t = 0.2, 0.4$ and 1.0. Using the FFT, data points are averaged over all possible combinations of x and y giving the same $r = |x-y|$ to improve the signal. As the flow time increases,

FIG. 1 (color online). The correlator $-\langle q(x)q(y) \rangle$ at the flow times $a^2t = 0.2$ (circles), 0.4 (triangles) and 1.0 (crosses). Data at $\beta = 4.17$, $am_{ud} = 0.007$ and $am_s = 0.040$ are presented.

¹A similar method was applied in a quenched study to extract the “pseudoscalar glueball mass” [15]. There are other viable definitions of the smearing as used in previous works to probe the topological structure of the QCD vacuum [16–19].

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the statistical fluctuation of the correlator becomes milder, while the region at small $|x - y|$ is distorted. We therefore need to find a region of t where the correlator has sufficiently small noises to find the signal while it is not distorted by the smearing of the YM gradient flow.

The data for $C(|x - y|)$ show a cleaner signal than the conventional zero-momentum projection, $\sum_{\vec{x}} \langle q(x)q(y) \rangle$, because of the average in all four-dimensional directions. The η' meson mass is extracted by fitting the data to the function of a single boson propagation:

$$f(r, m_{\eta'}) = A \frac{K_1(m_{\eta'} r)}{r}, \quad (3)$$

where $r = |x - y|$, K_1 is the modified Bessel function, and A is an unknown constant, which depends on the flow time t .

In order to determine the fitting range, we define a local “effective mass” $m_{\text{eff}}(r)$ by numerically solving $f(r + \Delta r, m_{\text{eff}}(r))/f(r, m_{\text{eff}}(r)) = C(r + \Delta r)/C(r)$. We set the interval to be $\Delta r = 1/2$, and the data of $C(r)$ in the range $[r, r + \Delta r]$ are averaged. As shown in Fig. 2, a reasonable plateau is found for $m_{\text{eff}}(r)$ around $r \sim 8-12$ (>0.6 fm) at $t = 1$ ($\sqrt{8t} \sim 0.2$ fm).

Figure 3 shows the η' meson mass obtained by fitting in the range $[8, 12]$ as a function of $\sqrt{8t}$. The data around $\sqrt{8t} \sim 0.2$ fm are stable. At larger smearing lengths $\sqrt{8t} \gtrsim 0.3$ fm, we observe a large distortion of the data. We take the data at $\sqrt{8t} = 0.2-0.25$ fm (filled symbols in Fig. 3) for our results.

We plot all the results in Fig. 4 as a function of the square of the pion mass m_π . We find that the dependence on the quark masses, as well as on V and a , is mild. We therefore perform a global fit of our data to a linear function $m_{\eta'}^{\text{phys}} + C_a a^2 + C_{ud}[m_\pi^2 - (m_\pi^{\text{phys}})^2] + C_s[(2m_K^2 - m_\pi^2) - \{2(m_K^{\text{phys}})^2 - (m_\pi^{\text{phys}})^2\}]$, where $m_{\eta'}^{\text{phys}}$, C_a , C_{ud} and C_s are taken as free

FIG. 2 (color online). The effective mass $m_{\text{eff}}(r)$ for the data with several flow times. Results for the $\beta = 4.17$ $am_{ud} = 0.007$ and $am_s = 0.040$ ensemble are shown.

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FIG. 3 (color online). The flow-time dependence of the η' meson mass. The data at various sea quark masses and β values are shown, as specified in the legend. The filled symbols represent our data taken for the central values.

parameters and $m_{\pi/K}^{\text{phys}}$ denotes the experimental value of the pion/kaon mass. As shown by the lines (which are shown for higher m_s only) in Fig. 4, we find that our linear function fits the lattice data reasonably with $\chi^2/(\text{degrees of freedom}) \sim 1.6$.

Because of possible bias in the topological charge sampling, the η' correlator may not decay exponentially but become a constant at long distances [27]. In each topological sector Q , it is predicted as [28]

$$\langle q(x)q(y) \rangle^Q \sim \frac{1}{V} \left(\frac{Q^2}{V} - \chi_t \right) \quad \text{at large } |x - y|. \quad (4)$$

The typical size of the constant term χ_t/V is 100–1000 times smaller than $|\langle q(x)q(y) \rangle|$ in our fitting range, which

FIG. 4 (color online). The extracted η' meson mass from each gauge ensemble. The three fit lines (representing the same linear fit function at three values of a) are shown for higher m_s 's at each β .

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is consistent with the fact that this observable shows no strong correlation to the global topological charge Q .

We also estimate that the finite volume effect on our observable is negligible, since the η' meson propagator implies $\exp(-m_{\eta'}L) \sim 3 \times 10^{-6}$ even at our lightest m_{ud} . Our data on a larger lattice $48^3 \times 96$, which are statistically consistent with those on the smaller lattice, support this assumption.

Since m_{ud} and m_s are nondegenerate, the flavor-singlet channel does not correspond to the mass eigenstate, and a mixing with the flavor nonsinglet channel is expected, which is the $\eta - \eta'$ mixing. We estimate the size of the η meson contribution to the flavor-singlet channel by modifying the fit function as

$$\frac{A}{r} K_1(m_{\eta'} r) \rightarrow \frac{A}{r} [e^{2m_{\eta'}^2 t} m_{\eta'} K_1(m_{\eta'} r) + e^{2m_{\eta}^2 t} m_{\eta} K_1(m_{\eta} r) \tan^2 \theta], \quad (5)$$

where θ is the mixing angle and m_{η} denotes the η meson mass. Note that the factors $e^{2m_{\eta'}^2 t}$ and $e^{2m_{\eta}^2 t}$ come from the effect of the YM gradient flow smearing. As a phenomenological estimate for m_{η} , we use $\sqrt{m_{\eta_s}^2(m_{ud} + 2m_s)/(3m_s)}$ where m_{η_s} is the (unphysical) mass of the connected pseudoscalar correlator of strange and anti-strange quarks [29]. We compare the fit curves with different fixed values of θ as shown in Fig. 5. As θ increases the quality of the fit becomes worse, especially at long distances. Thus, our data suggest a small mixing angle $|\theta| \lesssim 10^\circ$, and this tendency is seen at all our simulated parameters (the sign of θ is not relevant for this conclusion). The small mixing angle is consistent with the estimates from the quark model, $\theta = -25^\circ - -10^\circ$ [30]. In our simulations, θ is likely to be smaller than these phenomenological values since our simulated m_{ud} is closer to m_s . We confirm that the fit results with the fixed value of $\theta = 10^\circ$ are consistent with those with $\theta = 0$ within the statistical errors, although there exists a tendency that the $m_{\eta'}$ meson mass becomes higher for $\theta \neq 0$. We take this $\sim +5\%$ deviation as the systematic error from the η meson mixing.

Finally, we examine the systematics in the chiral and continuum extrapolation. Since both of the m_{π} and a^2 dependences are mild, even if we totally ignore these dependences, the (constant) fit works well, giving a 8% different value of $m_{\eta'}^{\text{phys}}$ from the original linear fit, which is

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FIG. 5 (color online). Comparison of the fit curves at different inputs θ .

within the statistical error. We take this $\pm 8\%$ as the possible systematic error in the extrapolations.

Our final result at the physical point is

$$m_{\eta'} = 1019(119) \begin{pmatrix} +97 \\ -86 \end{pmatrix} \text{ MeV}, \quad (6)$$

which is consistent with the experimental value $m_{\eta'} = 957.78(6)$ MeV [30]. Here the first error is statistical, and the second is the systematic error from the mixing with the η meson and the chiral and continuum extrapolations (added in quadrature). From the same set of correlators we obtain the topological susceptibility χ_t , which will be presented elsewhere.

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