The topological objects near the chiral crossover transition in QCD

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We study the underlying topology of gauge fields in 2+1 flavor QCD with domain wall fermions on lattices of size $32^3 \times 8$, at and immediately above the chiral crossover transition. Using valence overlap fermions with exact index theorem, we focus on its zero modes for different choices of periodicity phases along the temporal direction. Our studies show that the zero modes are due to fractionally charged topological objects, the instanton-dyons. We further provide qualitative study of the interactions between those and compare with the available semi-classical results, finding remarkably accurate agreement in all cases.

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Introduction Chiral symmetry breaking and confinement are two of the most striking non-perturbative phenomena that explains the phase diagram of strongly interacting matter described by Quantum Chromodynamics (QCD). While increasing evidences point to the fact that interacting topological objects in QCD – monopoles, instantons, instanton-dyons are driving the corresponding phase transitions, quantitative understanding of their exact role still require a lot of work.

Historically, discussion of chiral symmetry breaking started from Nambu-Jona-Lasinio (NJL) model [1], in which hypothetical strong attraction between fermions have been introduced. Based on analogy to theory of superconductivity, it explained formation of effective quark masses and massless pions. Two decades later the instanton liquid model (ILM) [2] identified the non-perturbative interaction with the instanton-induced 't Hooft Lagrangian. Unlike the 4-fermion interaction in the NJL model, it is not always an attractive thus explicitly violating the $U_A(1)$ symmetry. The ILM also proposed another view on the chiral symmetry breaking, related with collectivization of the topological fermionic zero modes into the so called zero mode zone. Multiple numerical simulations of ensemble of interacting instantons were done, for a review see [3], which were able to reproduce point-to-point correlation functions corresponding to different mesons and baryons, known from phenomenology and lattice studies.

Relating these developments to confinement, it was shown in Ref. [4, 5] that the nonzero holonomy (or the average Polyakov loop which is the confinement order parameter) can split $SU(N_c)$ instantons into $N_c$ constituents, known as instanton-dyons or instanton-monopoles. Henceforth we refer to them as dyons for simplicity. Ensembles of dyons via mean-field methods were studied analytically [6–9] as well as numerically [10–12]. These works could reproduce both deconfinement and chiral phase transitions occurring at the same temperature in QCD, and also explain extra phase transitions in beyond QCD theories with modified quark periodicity phases by “jumps” of the zero modes, from one type of dyon to another.

Whether the resulting semi-classical theory can indeed provide accurate description of these phenomena, can be investigated only through first principles lattice gauge theory techniques. One of the early studies of the kind was done by Gattringer [13] who used QCD Dirac operator with two different temporal periodicity conditions on $SU(3)$ pure gauge configurations as a tool to locate dyons. These results reported the existence of dyons in gauge theories without fermions. Further lattice studies have been performed by Mueller-Preussker, Ilgenfritz and collaborators [14, 15], along similar lines. Clusters of local topological fluctuations were identified using a local definition of topological charge, from the eigenvectors of the valence Dirac operator with generalized periodicity conditions. Observed correlation between the topological clusters and local eigenvalues of the Polyakov loop provided further evidence for the presence of dyons in QCD vacuum.

This Letter continues these efforts and is aimed at a more detailed understanding of the topological structures in QCD with physical quark masses, near the chiral crossover transition. In particular, it is a first attempt towards quantifying the density and interactions between different species of dyons as a function of temperature. We use the so called overlap Dirac operator [18, 19], a particular realization of fermions on the lattice that has exact chiral invariance, and therefore an exact index theorem [20], as detailed in the next section. This allows us to unambiguously identify the fermionic zero-modes and relate them to the underlying topological structures. We track their location and space-time profiles, by varying the temporal periodicity conditions for the overlap Dirac operator. In the subsequent sections, we provide convincing evidence that these topological objects do indeed quite accurately correspond to expectations from the semi-classical theory of dyons.

Methodology The configurations used in this work are $2 + 1$ flavor QCD configurations generated by the
HotQCD collaboration [21] using Môbious domain wall discretization [22, 23] for fermions and Iwasaki gauge action. The Euclidean space-time torus (lattice) has \( N_s = 32 \) sites along the spatial directions and \( N_T = 8 \) sites along the temporal direction. The light and the strange quark masses are chosen to be physical corresponding to pion mass of 135 MeV. The typical spatial size of the lattice is \( \sim 4 \) fm, about four times the pion Compton wavelength. The temperature is defined by \( T = 1/(N_T a) \) where \( a \) is the lattice spacing, \( \sim 0.1 \) fm. These same configurations have been previously used to calculate the chiral crossover transition temperature \( T_c \) and investigate the \( U_A(1) \) breaking [21]. The pseudo-critical temperature was measured to be \( T_c = 155(9) \) MeV. The choice of Môbious domain wall fermions is crucial since it allows extremely accurate chiral symmetry on the lattice; its residual breaking is of the order of \( \sim 2 \times 10^{-3} \). We have chosen 5-6 statistically independent gauge configurations at each of the two temperatures \( T/T_c \sim 1.0, 1.08 \) respectively, where the expectation value of the Polyakov loop is intermediate between zero and unity. We have specifically selected configurations with topological charge \( |Q_{top}| = 1 \), the cleanest set-up to study both zero and non-zero modes. Since the main aim of the paper is to identify the topological objects generating these modes, rather than calculating some average observables that require sampling of different \( Q \) sectors, we think this choice is well justified.

Since the domain wall configurations have a small chiral symmetry breaking and does not satisfy an exact index theorem on the lattice, we used zero modes of valence overlap Dirac operator to detect the topological structures of these configurations. The overlap operator is defined as \( D = 1 - \gamma_5 \text{sign}(H_W) \) where the kernel of the sign function is \( H_W = \gamma_5 (M - a D_W) \), \( D_W \) being the massless Wilson-Dirac operator. \( M \) is the domain wall height which is chosen to be in the interval \( [0, 2] \) to simulate one massless quark flavor on the lattice. Recall that the overlap operator satisfies the Ginsparg-Wilson relation [24], \( \gamma_5 D^{-1} + D^{-} \gamma_5 = a \gamma_5 \) defining the ‘chiral invariance’ on a finite lattice. Furthermore it has an exact index theorem, even at finite lattice spacings [20] and hence its zero modes can be identified with the topological objects of the underlying gauge configurations.

**Detecting the precise nature of the topological objects** is done by varying temporal periodicity conditions for the fermion fields. We remind that the expectation value of the \( SU(3) \) Polyakov loop is described by three eigenvalues at spatial infinity, known as the “holonomy phases” \( \mu_i \), which divide the phase circle into 3 different sectors of angular sizes \( \nu_i = (\mu_i+1 - \mu_i)/(2\pi) \), \( i = 1, 2, 3 \). The masses of the three types of dyons are proportional to \( \nu_i \) and are called the \( M_1 \), \( L \) and \( M_2 \) dyons corresponding to \( \nu_{1,2,3} \) respectively. For \( SU(3) \) color group these phases in the confining phase are \( \mu_1 = 0, \mu_2 = 2\pi/3, \mu_3 = 4\pi/3 \) respectively, and therefore masses of all three types of dyons are the same. Since \( \sum \nu_i = 1 \), the sum of masses of three types of dyons makes the instanton action. Still the Dirac operator should only have one zero mode, per value of the topological charge \( Q \). This means that only one of the dyons actually has the zero mode: which one depends on the periodicity condition of the fermions on the Matsubara circle, \( \psi_f(\tau + \beta) = e^{i\beta} \psi_f(\tau) \). Specifically, it is the dyon within the angular sector \( \mu_i \) to \( \mu_{i+1} \) to which the fermion phase \( \phi \) belongs, that contains the zero mode. Now, if the topological constituents of the vacuum are a set of caloron i.e. finite-\( T \) instantons, changing \( \phi \) would not produce any changes in Dirac eigenstates. If on the other hand the vacuum consists of independent dyons, one would see “jumps” as \( \phi \) crosses \( \mu_i \) and moves from one angular sector to the next. Note that while fermion phases \( \phi \) are temperature independent, the holonomies \( \mu_i \) move converging to zero at high \( T \); therefore such jumps should lead to phase transition at a certain temperature.

We have numerically implemented the generalized periodicity condition for fermions by setting the gauge links along the temporal direction in \( D_W \) from \( U_A(\beta = 1/T) \rightarrow e^{i\beta} U_A(\beta) \). The phases are chosen to be \( \phi = -\pi/3, \pi/3, \pi \), latter corresponding to the usual anti-periodic Matsubara periodicity condition. The resulting sign function and the Ginsparg-Wilson relation was realized numerically as precise as \( 10^{-9} \) for our lattice configurations. We then calculated the first 6 eigenvalues and eigenvectors of the valence overlap Dirac operator on domain wall configurations using the Kalkreuter-Simma Ritz algorithm [25]. Our observables are two gauge invariant quantities, the wavefunction density \( \rho(x) = \sum_{a=1}^{3} \sum_{i=1}^{3} \psi_{a,i}^\dagger (x) \psi_{a,i}(x) \) and the chiral density \( \rho_5(x) = \sum_{a=1}^{3} \sum_{i,j=1}^{4} \psi_{a,i}^\dagger (x) \gamma_5 (i,j) \psi_{a,j}(x) \), defined in terms of the eigenvectors \( \psi \) of the overlap operator. In subsequent sections, by studying space-time profiles of the zero modes and the “jumps” of their positions for different periodicity conditions, we will identify the presence of dyons. The exact zero eigenmodes we study are well disentangled from the higher modes, making them completely insensitive to any ultra-violet fluctuations of the gauge fields. A more detailed study on the robustness of our results with respect to different lattice artifacts can be found in Ref. [26].

**Results:** As mentioned earlier, we focus on \( |Q| = 1 \) configurations, with one overlap fermion zero mode each, for 3 choices of the periodicity phase. The snap-shots of the eigenvalue density \( \rho(x, y) \) along two spatial directions exemplified in Fig. 1 provide extreme cases of well separated and strongly overlapping topological objects. These zero modes display rich underlying topological structures of the QCD vacua at finite temperatures, both at \( \sim T_c, 1.08 T_c \). The profiles for three different fermion periodicity phases \( \phi = \pi, -\pi/3 \) and \( \pi/3 \) are shown in red, green and blue colors respectively. The
left panel represents a case at $T \sim T_c$ when the observed topological objects are reasonably well separated in space, making their individual identification possible by changing the periodicity phase of the valence (overlap) fermion operator. The positions of the zero modes shift as the periodicity phases of fermions are changed. This provides us an evidence that the objects we observe are dyons. Next we study the vacuum profiles of two statistically independent QCD configurations at $1.08 T_c$, shown in the middle and the right panels of Fig. 1 respectively. In the middle panel, the fermion zero-modes can be seen to be localized at different spatial coordinates when the periodicity conditions are changed, like in the previous configuration near $T_c$. The configuration shown in the right panel shows a different limiting case where all three dyons are superimposed at the same location.

We compared the observed eigenmode density with the analytic expression for the dyon zero-mode density

$$\rho(x) = -\frac{1}{x^2} \frac{1}{(4\pi^2)} \frac{1}{\delta_m} f_x(\phi, \phi')$$

along four-vector $x$ as calculated in Ref. [17], with the function $f_x$ defined by

$$f_x(\phi, \phi') = 2\pi \delta(\phi - \phi')$$

Here $D_\phi = \frac{1}{x} \partial_\phi - \tau$ and the functional $r^2(x, \phi) = r_m^2(x)$, if the fermion periodicity phase $\phi \in [\mu_m, \mu_{m+1}]$ i.e. lies between the two neighboring holonomy phases. The delta function chooses dyons with different holonomy as evident from its definition, $\delta_m = \delta(\phi - \mu_m)|x_m - x_{m+1}|$. In fact the long-distance fall-off of the eigenvalue density $\rho(x)$ along any direction $x$ is controlled by the phases of the Polyakov loop $\mu_m$ and the distance between dyons. When the dyons are isolated and well separated from each other their long-distance fall-off is exponential in the difference between the periodicity phase $\phi$ and the nearest $\mu_m$.

In the case of well separated dyons, comparison with these analytic formulae is straightforward and success-
ful. But even in a strongly overlapping case, as depicted in the right panel of Fig. 1, we propose here a method which could be successfully used to distinguish between the two possibilities: whether it represents an isolated caloron with trivial holonomy (all $\mu_1, \mu_2, \mu_3 \to 0$, $\langle P \rangle = 1$), or closely superimposed dyons corresponding to non-trivial holonomy. To address this we show the eigendensity $\rho(x)$ along a spatial direction $x$ in Fig. 2 with the other 3 coordinates fixed at its maximum. The lattice data are compared to the density calculated analytically for both of these options, for which the corresponding Polyakov loop values were chosen to be $\langle P \rangle = 1$ (red curve) and $\langle P \rangle = 0.4$ (blue curve) respectively. The profile corresponding to $\langle P \rangle = 0.4$ is not symmetric, due to the pres-
ence of nearby dyons, while for $\langle P \rangle = 1$ it is symmetric about the maximum. We conclude that the long-distance fall-off of the density profile measured on the lattice is in better agreement with the blue rather than the red curve; so even the extreme case depicted in the right panel of Fig. 1 represents three overlapping dyons, rather than a caloron with trivial holonomy.

The robustness of the semi-classical correspondence to the QCD vacuum is tested in another contrasting scenario at $1.08 T_c$ when the fermion zero modes are well separated. In this case, the lattice result for the zero mode density $\rho(x, \tau)$ can provide a distinct indication for the distance between dyons. The $\rho(x, \tau)$ for phase angle $\phi = \pi/3$ measured on the lattice is shown in blue in Fig. 3. Again modeling this analytically using Eq. 1 with $\langle P \rangle = 0$ and placing the three dyons corresponding to $\phi = \pi/3, -\pi/3$ and $\pi$ respectively at coordinates $(0, 0, 0), (0.2/T, 0, 0)$ and $(-0.2/T, 0, 0)$, we obtained the profile shown in red in the same figure which mimics the lattice result quite well. While the shapes and the amount of overlap between the peaks varies across configurations studied here, we have not found any instance where these could not be explained by the semi-classical theory of dyons.

The near-zero profiles of the QCD Dirac operator The study of near-zero modes of the QCD Dirac operator can provide further insights on the interactions between topological constituents of QCD vacuum. If the density of topological objects is small or they are fairly dense but weakly interacting, in either case would lead to a very sparse eigenvalue density of near-zero modes. We look into the first near-zero mode for a configuration at $1.08 T_c$ presented earlier in the middle panel of Fig. 1. In order to extract maximum information out of the near-zero modes, their chiral densities are measured at two different periodicity phases $\phi = \pi$ and $\phi = \pi/3$ respectively, results of which are shown in Fig. 4. For $\phi = \pi$, we observe one pair of closely separated dyon and an anti-dyon. Changing to $\phi = \pi/3$ a more richer picture emerges; the dominant dyon that contributed to the zero mode has a prominent peak with positive chirality and atleast two distinct anti-dyon peaks are located near to it. These results have a very nice physical interpretation. Since the underlying gauge configurations were generated with anti-periodic Matsubara periodicity conditions for the fermions, the fermion determinant naturally suppressed those configurations which consisted of well separated $L$-dyons. In contrast configurations with well separated $M$-dyons (corresponding to the phase $\phi = \pi/3$ ) or $MM$ pairs are not suppressed. Moreover it is expected that at $T > T_c$ the $M$-dyons are lighter than the $L$-dyons and hence are more numerous. We next look at the near-zero mode profiles for the QCD configuration closer to $T_c$ for $\phi = \pi$ whose zero modes were observed earlier in the left panel of Fig. 1. The density of $LL$ dyons is believed to increase as one approaches $T_c$ leading to collectivization of near-zero modes of the QCD Dirac operator. This is also what we observe in Fig. 5. Unlike calorons, dyons interact directly with the holonomy potential. Increasing density of dyons near $T_c$ is long suspected to provide a strong back-reaction to overcome the perturbative Gross-Pisarski-Yaffe potential [27] for the Polyakov loop and drive it towards its confining value. This first principles observation of collectivization in realistic QCD configu-
rations would eventually help towards an understanding of the mechanism of confinement.

**Summary** Unlike various versions of “cooling”, the fermion eigenmode method we use reveals the underlying topological objects in QCD configurations without any modifications. For the first time, we applied this to QCD configurations with physical quarks and with chiral symmetry realized to a good precision on the lattice. Our choice of valence overlap fermions with an index theorem allowed us to study the properties of topological objects at temperatures $T_c$ and $1.08 T_c$, focusing on its zero modes. Changing the Matsubara periodicity phases of the (overlap) fermions to $\phi = \pi, \pi/3, -\pi/3$, we identified all three types of dyons by observing their locations and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles. The other advantage of this method is that no gauge fixing is required to detect dyons and their density profiles.

We extensively studied different possible situations, ranging from widely separated dyons to fully overlapping ones. By quantitatively comparing their spacetime profiles with the available analytic formulae for well separated and, most importantly, partially overlapping dyons, we found in all cases a good agreement, with deviations not exceeding $\sim 10\text{-}20\%$ level. This is remarkable accuracy for a semi-classical theory, taking into account the fact that the typical action per dyon is $S \sim 3\text{-}4 \hbar$ and naively, relative fluctuations are expected to be $O(1/S)$.

Furthermore we could extract rich qualitative information about the density and interactions between dyons from a detailed study of chiral density profiles of the quark near-zero modes. At $T_c$, the density of the $L$-dyons increases and the attractive interaction between the $LL$ pairs lead to collective manifestation of near-zero modes. As the temperature is increased, the density of dyons decreases resulting in a sparsely populated near-zero eigendensity of the QCD Dirac operator. We are continuing this work towards a more quantitative measurement of the density and the correlations between the dyons in a forthcoming publication [26].

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