Calorons and localization of quark eigenvectors in lattice QCD

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We analyze the localization properties for eigenvectors of the Dirac operator in quenched lattice QCD in the vicinity of the deconfinement phase transition. Studying the characteristic differences between the $Z_3$ sectors above the critical temperature $T_c$, we find indications for the presence of calorons.

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One of the most discussed topics in hadron physics is the chiral phase transition of QCD, and the microscopic processes connected with it. Many current and planned experiments are at least partially motivated by the hope that they will shed some light on the issues involved.

In this contribution we study the localization properties of the lattice Dirac operator in the neighborhood of the chiral phase transition. We are motivated by the fact that one of the most popular pictures of the phase transition relates it to the properties of QCD instantons and anti-instantons (see e.g. Ref. [1]). The origin of this connection is the following observation: For each isolated instanton or anti-instanton there exists a localized zero mode of the Dirac operator. For a liquid of instantons and anti-instantons these zero modes should be perturbed to form a band of small eigenvalues. At higher temperatures it is thought that instantons and anti-instantons may pair to form molecules, and that the associated modes will no longer have particularly small eigenvalues, but instead become an inconspicuous part of the bulk spectrum.

The Banks-Casher formula [2]:

$$\langle q\bar{q} \rangle = -\frac{\pi \rho_{\text{Dirac}}(0)}{V},$$

relates the chiral condensate $\langle q\bar{q} \rangle$ to $\rho_{\text{Dirac}}(0)$, the density of Dirac eigenvalues at zero, evaluated in the (large) volume $V$. Thus we expect that if the instantons and anti-instantons form a liquid, chiral symmetry will be broken, but that if they form instanton–anti-instanton molecules, chiral symmetry will be restored.

If this interpretation is correct the chiral phase transition should reflect itself also in a characteristic change of the localization properties of the lowest Dirac eigenvectors. This is the main motivation for our studies.

In addition we are interested in comparing our lattice results with predictions from random matrix theory (RMT). Such a comparison allows us to distinguish generic from QCD-specific properties. Similar studies were performed before in Ref. [3]. In this paper, however, the authors analyzed a specific instanton-liquid approximation to QCD while we study lattice QCD.

As usual, we simulate a finite-temperature system by working on a lattice with $L_t < L_s$, where $L_t$ ($L_s$) is the temporal (spatial) extent of the lattice. All boundary conditions are antiperiodic. The temperature is given by $aT = 1/L_t$ with the lattice spacing $a$. We fix $L_t = 6$ and vary $a$ (and hence $T$) by changing $\beta = 6/g^2$.

We work in the quenched approximation with staggered fermions, i.e. with the Dirac operator

$$D = \sum_{\mu=1}^{4} \frac{1}{2a} \alpha_\mu(x) \left[ \delta_y, x+\hat{\mu} U_\mu(x) - \delta_y, x-\hat{\mu} U_\mu^\dagger(y) \right],$$

where $\alpha_\mu(x) = (\pm 1)^{x_1+\ldots+x_{n-1}}$ and the $U_\mu$ are the link variables. The eigenvalues of $D$ come in pairs of $\pm \lambda$, so we can restrict ourselves to positive eigenvalues in the following. In the continuum limit this action corresponds to four quark flavors. From now on we set $a$ to 1.

Quenched QCD has an additional $Z_3$ symmetry of the gauge sector, which is spontaneously broken in the deconfined phase [4]. In the confined phase the expectation value of the Polyakov loop $P$ is zero, whereas in the deconfined phase $\vert P \vert$ acquires an expectation value, and the phase of $P$ clusters around the values $\theta_P = \arg(P) = 0, \pm 2\pi/3$. The fermion action does not share the $Z_3$ symmetry, so fermionic quantities can depend on the $Z_3$ sector. It was found in Ref. [4] that the chiral condensate computed from the configurations with $\theta_P = 0$ vanishes above $T_c$ as expected. For $\theta_P = \pm 2\pi/3$ it remains finite in a certain temperature range above $T_c$. This behavior can be understood in Nambu-Jona-Lasinio models [5] and in RMT [6]. The point is that the boundary conditions of the Dirac operator are not invariant under $Z_3$ transformations, and for $\theta_P = \pm 2\pi/3$ the new boundary conditions lead to a decrease of the Dirac eigenvalues [8]. According to the Banks-Casher relation, Eq. [1], this implies that the condensate will disappear only for larger temperatures, i.e. the transition temperature is higher for these sectors. For phenomenological comparisons one should use the $\theta_P = 0$ sector as this one is energetically favored for dynamical fermions.
Large temperatures correspond to a small extension of the lattice in the temporal direction. The periodic boundary conditions for the gauge fields thus imply that the field equations have solutions with nontrivial topology which look rather like an instanton chain. Such configurations, called calorons, have been the topic of intense investigations. The index theorem tells us that the continuum Dirac operator has a chiral zero mode in a caloron field, so we will search for calorons by looking at the chiral and localization properties of the eigenvectors of the low-lying eigenvalues of $D$. To calculate the eigenvalues and eigenvectors we used the Arnoldi method as implemented in Ref. [10]. This method allows us to choose the number of vectors we used the Arnoldi method as implemented in Ref. [10]. This method allows us to choose the number of eigenvectors we used the Arnoldi method as implemented in Ref. [10]. This method allows us to choose the number of eigenvectors we used the Arnoldi method as implemented in Ref. [10].

As a measure of the localization of our quark eigenvectors $\psi^\alpha(x)$ ($\lambda$ is the Dirac eigenvalue, $\alpha$ a color index) we use a gauge-invariant inverse participation ratio (IPR), defined by

$$I_2 = V \left[ \sum_x p_\lambda(x)^2 \right] / \sum_x p_\lambda(x)^2 ,$$

where $V$ is the number of lattice sites and $p_\lambda(x)$ is the gauge-invariant probability density

$$p_\lambda(x) = \sum_{\alpha=1}^{N_\alpha} |\psi^\alpha_\lambda(x)|^2 .$$

For a completely delocalized state (all $p_\lambda(x)$ the same) one finds $I_2 = 1$, whereas a state localized on a single lattice site (only one non-zero $p_\lambda(x)$) would have $I_2 = V$. (The staggered fermions' chiral symmetry means that in fact an eigenstate can never be completely localized, since all eigenstates must have half their probability on even sites, and half on odd.) $I_2$ is also a measure of the standard deviation of $p_\lambda(x)$,

$$I_2 - 1 = \frac{1}{V P_\lambda^2} \sum_x \left[ p_\lambda(x) - \bar{p}_\lambda \right]^2 .$$

Chiral RMT predicts that the average value of $I_2$ is

$$\langle I_2 \rangle = \frac{(N_c + 1) V}{N_c V + 2} + \frac{1}{N_c} \quad \text{for} \ N_c \geq 3 .$$

To elucidate the relevance of the IPR let us note that in condensed matter physics the size of the IPR decides e.g. whether a disordered mesoscopic sample is a metal ($I_2$ close to the RMT prediction) or an insulator ($I_2$ large).

We have investigated the behavior of $I_2$ on finite temperature lattices, on both sides of the deconfinement phase transition, which lies at $\beta \approx 5.89$ for $L_t = 6$ in the thermodynamic limit [11].

Slightly above $T_c$ the localization properties show characteristic differences for the different $Z_3$ sectors. In the real sector the effect of localization is strongly pronounced while it is nearly absent in the $\theta_P = \pm 2\pi/3$...
sectors where chiral symmetry is still broken for these temperatures. This is illustrated in Figs. 3 and 4. A difference between localization in the different sectors tells us immediately that the eigenstates must be extended in the time direction, because an eigenstate localized in time would be unaffected by a $Z_3$ transformation.

We studied these characteristic differences for high temperatures in more detail and found features which suggest that they can be attributed to the effects of calorons, as we shall now explain.

Harrington and Shepard found exact SU(2) instanton solutions at finite temperature [3], which they called calorons (for a review see Ref. [12]). Their solution consists of a one-dimensional chain of instantons, with a periodic repeat at a distance $1/T$. There is a single physically relevant parameter, $RT$, which gives the instanton radius $R$, relative to the scale set by the temperature. When $RT \ll 1$ the solution looks like an isolated instanton, but when $RT \sim 1$ finite temperature effects become significant. This instanton chain satisfies the 't Hooft ansatz [13], so the techniques described in Ref. [14] can be used to find the fermionic zero modes [13]. For small $RT$ these look like the zero modes of an isolated instanton, but as $RT$ increases, the modes become extended in time, though they remain localized in space. These SU(2) solutions can easily be embedded in SU(3), leading to solutions which correspond to the $\theta_P = 0$ sector. To investigate the other sectors, we need solutions where the time-like Polyakov loop has a non-zero phase at space-like infinity. We can construct such solutions either by adding a constant $A_4$ background field with a color that commutes with the SU(2) subgroup containing the caloron, or by choosing the fermion field boundary condition appropriately. In either case the fermionic zero modes are readily constructed. One can also find pure SU(2) solutions with a Polyakov loop background [16]. It would be interesting to study the relationship between these solutions and the solutions found by embedding the Harrington-Shepard solution in SU(3).

The localization of the embedded caloron’s fermion zero mode depends heavily on the $Z_3$ sector. Asymptotically the modes fall off like

$$|\psi|^2 \propto \exp[-2(\pi - |\theta_P|) rT]/r^2$$

where $r$ is the three-dimensional distance from the caloron axis. (At $\theta_P = 0$, this agrees with the behavior given in Ref. [12].) This is unlike the case of a single instanton, which has $|\psi|^2$ which drops off like a power of $r$. We see from Eq. (6) that the correlation length for the zero mode is smallest in the real sector ($\theta_P = 0$), and that the complex $Z_3$ sectors ($\theta_P = \pm 2\pi/3$) have modes in which the radius is about three times greater, and so they occupy a much larger volume. It is thus tempting to assume that the strong difference between the localization properties in the $Z_3$ sectors is due to the fact that our lattice configurations contain calorons. If so, the localization in four dimensions should show the characteristic string-like pattern discussed above.

In Fig. 4 the localization itself and the local density of the expectation value of $\gamma_5$ are shown for a highly localized state in the $\theta_P = 0$ sector (mode 1 of Figs. 1 and 2). To plot the complete four-dimensional lattice we have introduced the two coordinates $i = x + 12t$ and $j = y + 12z$ with the Euclidean lattice coordinates $x, y, z = 0, 1, 2, \ldots, 11$ and $t = 0, 1, \ldots, 5$. This coordinate system represents the lattice as a $6 \times 12$ array of $x$-$y$ slices, which generates the approximately periodic structure visible in the plot. From the upper plot, we see that the state is indeed spatially localized, but extended in

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**References**

1. [Ref. 1]
2. [Ref. 2]
3. [Ref. 3]
4. [Ref. 4]
5. [Ref. 5]
6. [Ref. 6]
7. [Ref. 7]
8. [Ref. 8]
9. [Ref. 9]
10. [Ref. 10]
11. [Ref. 11]
12. [Ref. 12]
Modes related to instantons and calorons were recently investigated in lattice QCD with dynamical fermions [7]. While the results below $T_c$ are consistent with expectations based on an instanton liquid picture, the interpretation of the observations above $T_c$ appears to be less straightforward.

Let us summarize: We have analyzed the localization properties of quark eigenstates in quenched lattice QCD. By concentrating on the low eigenvalues we could characterize semiclassical properties of the gauge field configurations without any cooling. (For investigations using cooling, see e.g. Ref. [5].) For temperatures above $T_c$ we found isolated modes with definite handedness which show all the properties of fermion states associated with calorons, in particular localization in space but not in time.

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\[ \langle \gamma_5 \rangle \]

FIG. 4. A ‘caloron’ state (mode 1 of Figs. 1 and 2) on a $12^3 \times 6$ lattice for $\beta = 6.1$ in the $\theta_p \approx 0$ sector. We have introduced the coordinates $i = x + 12t$ and $j = y + 12z$ with the lattice coordinates $x, y, z = 0, 1, \ldots, 11$ and $t = 0, \ldots, 5$. The gauge-invariant density is plotted above, the expectation value of $\gamma_5$ below. Both show localization in space but not in time.

The lower plot demonstrates that the eigenstate in question is an approximate chiral eigenstate. A continuum caloron would possess an exact chiral eigenstate. Unfortunately, staggered fermions exhibit only part of the continuum chiral invariance, which is the reason why we do not find perfect $\gamma_5$ eigenstates. It would therefore be very interesting to repeat these studies with Ginsparg-Wilson fermions which have much better chiral properties.

The corresponding pictures for mode 2 look similar to Fig. 3. The width of the mode is, however, noticeably larger than that of mode 1. Mode 3 serves as an example for a mode with low $\langle \gamma_5 \rangle$, high $f_2$, and an eigenvalue which lies in the bulk of the spectrum. Although $\langle \gamma_5 \rangle$ is small, the $\langle \gamma_5 \rangle$-density has a region of large positive values right next to a region where the density is large and negative. This suggests mode 3 might be an instanton–anti-instanton molecule.