Probing the chiral phase transition of $N_f = 2$ clover fermions with valence overlap fermions

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FOR THE DIK-COLLABORATION

Overlap fermions are a powerful tool for investigating the chiral and topological structure of the vacuum and the thermal states of QCD. We study various chiral and topological aspects of the finite temperature phase transition of $N_f = 2$ flavours of $\mathcal{O}(a)$ improved Wilson fermions, using valence overlap fermions as a probe. Particular emphasis is placed upon the analysis of the spectral density and the localisation properties of the eigenmodes as well as on the local structure of topological charge fluctuations in the vicinity of the chiral phase transition. The calculations are done on $16^3 \times 8$ lattices generated by the DIK collaboration.

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1. Introduction

Since overlap fermions have an exact chiral symmetry on the lattice, they are an appropriate tool to investigate the chiral phase transition. Simulations involving the effects of dynamical overlap sea quarks are just becoming possible now, but as they are still numerically extremely demanding on realistic lattices, we use a hybrid approach by implementing the overlap action for the valence quarks on dynamical configurations generated with \( N_f = 2 \) flavours of \( \bar{O}(a) \) improved Wilson sea quarks.

As the lattice spacing, \( a \), for dynamical fermions is connected to both the coupling constant \( \beta \) and \( \kappa_{\text{sea}} \), increasing the temperature \( T = 1/(N_a a) \) across the transition is affected by an increase in \( \kappa_{\text{sea}} \) at fixed values of the coupling, \( \beta \), and time-extent, \( N_a \), of the lattice. In order to probe the topological properties of dynamical gauge fields in the vicinity of the phase transition, we concentrate on the values \( \kappa_{\text{sea}} = 0.1343 \), 0.1348 and 0.1360 corresponding to \( T/T_c = 0.98 \), 1.06 and 1.27, respectively, at fixed \( \beta = 5.2 \) on \( 16^3 \times 8 \) lattices generated by the DIK-collaboration [3]. The lattice spacing is approximately \( a = 0.12 \text{ fm} \). We use \( O(200) \) configurations for each value of \( \kappa_{\text{sea}} \). The transition point \( \kappa_c \) can be identified as the point where the Polyakov loop susceptibility \( \chi = N_f^2 \langle L^2 \rangle - \langle L \rangle^2 \), with the Polyakov loop \( L(\vec{s}) = \frac{1}{4} \text{Tr} \prod_{\alpha=1}^{N_f} U_4(\vec{s},s_\alpha) \), assumes its maximum. Recent work of the DIK-collaboration on \( 16^3 \times 8 \) lattices at \( \beta = 5.2 \) gave \( T_c = 212(2) \text{ MeV} \), corresponding to \( \kappa_c = 0.13444(6) \) [3].

2. Density and locality of the eigenmodes of the overlap operator

The spontaneous breaking of chiral symmetry by the dynamical creation of a nonvanishing chiral condensate, \( \langle \bar{\Psi}\Psi \rangle \), is related to the spectral density \( \rho(\lambda) \) of the Dirac operator near zero by the Banks-Casher relation \( \langle \bar{\Psi}\Psi \rangle = -\frac{2}{\pi} \rho(0) \). Using the Arnoldi-algorithm, we compute the 50 lowest eigenvalues on every configuration. To smooth the configurations we perform 1 step of APE-smearing, using the smearing coefficient \( \alpha = 0.45 \). In Fig. 3, we plot the spectral density. One can clearly see a nonvanishing chiral condensate in the chirally broken phase at \( \kappa_{\text{sea}} = 0.1343 \) below the phase transition and a large gap in the spectrum at \( \kappa_{\text{sea}} = 0.1360 \) in the symmetry restored phase. However, at \( \kappa_{\text{sea}} = 0.1348 \), a value which was determined by the Polyakov-loop method to be above the transition, we find a nonvanishing tail of small eigenvalues extending down to zero.

A useful measure to quantify the localisation of eigenmodes [5] is the inverse participation ratio \( I = V \sum_x \rho(x)^2 \), with the scalar density \( \rho(x) = \psi_\lambda^\dagger(x) \psi_\lambda(x) \) for normalised eigenfunctions \( \sum_x \rho(x) = 1 \). While \( I = V \) if the density has support only on one lattice point, \( I \) decreases as the density becomes more delocalised, reaching \( I = 1 \) when the density is maximally spread on all lattice sites. Fig. 3 shows the IPR’s for all configurations as a function of the modulus of the eigenvalue below and above the phase transition. One can see that in both cases the zero modes and the first non-zero eigenmodes are highly localised, while the mean IPR for the highest computed eigenvalues is approximately 1.3.

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1. Our results on the vacuum structure for \( T = 0 \) quenched configurations are presented in the talk by Y. Koma [3] at this conference.

2. For our implementation of the overlap operator see Ref. [3]. Also here we use \( \rho = 1.4 \) and stereographically project the eigenvalues.
3. The local structure of topological charge fluctuations

The topological charge density for any \( \gamma_5 \)-Hermitean Dirac operator satisfying the Ginsparg-Wilson relation is defined as \([6]\):

\[
q(x) = \frac{1}{2} \text{Tr} \gamma_5 D(x,x), \quad Q = \sum_x q(x). \tag{3.1}
\]

To compute the topological charge density, we use two different approaches \([7, 8]\). In the first approach, we directly calculate the trace of the overlap operator according to equation Eq. (3.1). This is a computationally very demanding task and is therefore performed on only 5 configurations for each \( \kappa_{sea} \). The “full” density computed in this way includes charge fluctuations at all scales. The second technique involves the computation of the topological charge density based on \( O(50) \) low lying modes of the overlap Dirac operator. Using the spectral representation of the Dirac operator, the eigenmode expansion of the topological charge density reads

\[
q_\lambda(x) = - \sum_\lambda (1 - \frac{\lambda}{2}) c_\lambda(x), \quad c_\lambda(x) = \psi_\lambda^+(x) \gamma_5 \psi_\lambda(x). \tag{3.2}
\]

Truncating the expansion acts as an ultraviolet filter by removing the short-distance fluctuations from \( q(x) \). Note that the topological charge \( Q = \sum_x q_\lambda(x) \) is not affected by the level of truncation.
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Figure 3: Isosurfaces of topological charge density with $|q(x)|/q_{\text{max}} = 0.1, 0.2, 0.3, 0.4$, with red (green) surfaces indicating positive (negative) charges in one timeslice of a configuration with $\kappa_{\text{red}} = 0.1343$. The upper (lower) pictures are based on the full (eigenmode truncated) density.

Reflection positivity, i.e. positivity of the metric in Hilbert space, demands that the topological charge correlator is negative [9]

$$\langle q(x)q(y) \rangle \leq 0, \quad r > 0, \quad (3.3)$$

where $r = |x - y|$ is the Euclidean distance. Since overlap fermions are not ultralocal, the fermion action is not strictly reflection positive. Therefore, analysing dynamical or quenched lattices with valence overlap fermions, one may expect a positive core and a negative tail of $C_q(r)$ [1, 10]. This will be washed out when a finite UV filter is applied.

Let us first consider the local structure of the topological charge fluctuations, studying sign coherent clusters formed by connected neighbours $x_i$ with $|q(x_i)| > q_{\text{cut}} = 0.1 \ldots 0.4 q_{\text{max}}$, where $q_{\text{cut}}$ is a cutoff value to be varied at will. To give a picture of the spatial distribution of the topological charge density, isosurface plots with $q(x) = \pm q_{\text{cut}}$ are shown in Fig. 3.

It is obvious that the UV cutoff in the topological density results in a completely different structure actually seen by the lowest modes. This is also reflected in Fig. 3 which shows the topological charge correlator Eq. (3.3) in terms of the truncated density. We take 50 modes into account, which seems not to be sufficient to generate the negative tail of the correlator [1]. Since hypercubic rotation symmetry could be broken we plot the correlator as a function of the Euclidean distance $r$ and the temporal distance $t$. The UV truncated correlator represents mainly size, shape and temperature dependence of the clusters seen in the lower row of Fig. 3. We see a slightly more negative correlation developing in the high-temperature phase.

Further investigating the full density, we show in Fig. 3(a) and (b) that the number of clusters reaches a maximum at a moderate cutoff value, while for a cutoff as low as $q_{\text{cut}} = 0.1 q_{\text{max}}$ there

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3Movies are available at [http://www.cip.physik.uni-muenchen.de/~weinberg/topdens/](http://www.cip.physik.uni-muenchen.de/~weinberg/topdens/).
are 2 totally dominating oppositely charged clusters with a fractional volume of around 50% each.\footnote{The maximal number of clusters of the truncated density is an order of magnitude smaller.} The fractional volume and the total charge of the clusters ordered by their size are plotted in Fig. 3. Studying the point-to-point correlation of the largest clusters based on the full charge density, we find that the clusters start to percolate at $q_{\text{cut}} = 0.2 (0.25) q_{\text{max}}$ for $\kappa = 0.1343 (0.1360)$. Fig. 5(c) shows the maximum of the minimal distance between each point of the largest cluster and every point of the second largest one. The small value for low cutoffs in $q$ implies that the 2 dominating clusters are tangled and intertwined in a complex way.

A preliminary dimensional analysis indicates that we are rediscovering for the full density the picture of 2 dominating approximately 3D sign coherent clusters \cite{11} at low cutoffs also at finite $T$, whereas we see 1D highly charged small clusters at high thresholds. This picture means that the QCD vacuum model with 4D coherent (anti)instantons with a typical instanton radius of $0.3 - 0.4$ fm is strongly modified by quantum fluctuations. The eigenmode-truncated density is more compatible with the conventional multiple-lump picture. Apart from the topological susceptibility which is strongly suppressed in the chiral-symmetry restored phase, only quantitative structural differences between the phases are seen so far.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4}
\caption{The topological charge correlator using 50 eigenmodes on $\mathcal{O}(200)$ configurations.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5}
\caption{The total number of clusters of full density (a), the fractional size of the largest cluster (b) and the distance between the 2 leading clusters (c) depending on the cutoff value.}
\end{figure}
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Figure 6: Fractional volume (upper plot) and total charge (lower plot) of the clusters of full charge sorted by their size for $q_{\text{cut}} = 0.10 \ q_{\text{max}}$ (left) and $0.40 \ q_{\text{max}}$ (right) for one configuration with $\kappa_{\text{sea}} = 0.1343$.

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References

[1] Y. Koma et al., Localization properties of the topological charge density and the low lying eigenmodes of overlap fermions, PoS(LAT2005)300 (these proceedings) [hep-lat/0509164].

[2] DIK Collaboration, V. G. Bornyakov et al., Finite temperature QCD with two flavors of non-perturbatively improved wilson fermions, Phys. Rev. D71 (2005) 114504 [hep-lat/0401014].

[3] Y. Nakamura et al., Critical temperature in QCD with two flavors of dynamical quarks, PoS(LAT2005)157 (these proceedings) [hep-lat/0509122].

[4] QCDSF-UKQCD Collaboration, D. Galletly et al., Quark spectra and light hadron phenomenology from overlap fermions with improved gauge field action, Nucl. Phys. Proc. Suppl. 129 (2004) 453–455 [hep-lat/0310028].

[5] MILC Collaboration, C. Aubin et al., The scaling dimension of low lying Dirac eigenmodes and of the topological charge density, [hep-lat/0410024].

[6] P. Hasenfratz, V. Laliena and F. Niedermayer, The index theorem in QCD with a finite cut-off, Phys. Lett. B427 (1998) 125–131 [hep-lat/9801021].

[7] I. Horvath et al., On the local structure of topological charge fluctuations in QCD, Phys. Rev. D67 (2003) 011501 [hep-lat/0203027].

[8] I. Horvath et al., Low-dimensional long-range topological charge structure in the QCD vacuum, Phys. Rev. D68 (2003) 114505 [hep-lat/0302003].
[9] E. Seiler, *Some more remarks on the Witten-Veneziano formula for the $\eta'$ mass*, Phys. Lett. **B525** (2002) 355–359 [hep-th/0111125].

[10] I. Horvath et al., *The negativity of the overlap-based topological charge density correlator in pure-glue QCD and the non-integrable nature of its contact part*, Phys. Lett. **B617** (2005) 49–59 [hep-lat/0504005].

[11] I. Horvath et al., *Inherently global nature of topological charge fluctuations in QCD*, Phys. Lett. **B612** (2005) 21–28 [hep-lat/0501025].