Quenched QCD at finite temperature with chiral Fermions

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We study physics at temperatures just above the QCD phase transition ($T_c$) using chiral (overlap) Fermions in the quenched approximation of lattice QCD. Exact zero modes of the overlap Dirac operator are localized and their frequency of occurrence drops with temperature. This is closely related to axial $U(1)$ symmetry, which remains broken up to $2T_c$. After subtracting the effects of these zero modes, chiral symmetry is restored, as indicated by the behavior of the chiral condensate ($\langle \bar{\psi} \psi \rangle$). The pseudoscalar and vector screening masses are close to ideal gas values.

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With new results from the Brookhaven heavy-ion collider appearing thick and fast [4], the time seems ripe for making a concerted effort to understand the dynamics of the high-temperature phase of quantum chromodynamics, namely the quark-gluon plasma. There are several puzzles that seem to have resisted a decade of efforts to understand them. The one we focus on involves the static screening of certain excitations of the plasma.

It has long been understood that the screening of currents in a plasma would give us information on its excitations. Currents with certain quantum numbers excite mesons from the vacuum at low temperatures, and should exhibit deconfinement related changes above the QCD phase transition temperature ($T_c$) [3]. Detailed studies have shown that this indeed does happen in the vector, and axial-vector channels: the screening above $T_c$ is clearly due to nearly non-interacting quark anti-quark pairs in the medium [3]. On the other hand, the scalar and pseudo-scalar screening masses show more complicated behavior— strong deviations from the ideal Fermi gas, and a strong temperature dependence. This puzzling behavior is generic— it has been seen in quenched [8] and dynamical simulations with two [13] and four flavors [11] of staggered quarks, as well as with Wilson quarks [10]. This is the puzzle that we address and solve in this letter.

The new technique we bring to bear on this problem is to use a version of lattice Fermions called overlap Fermions [14]. It has the advantage of preserving chiral symmetry on the lattice for any number of massless flavors of quarks [13]. This is in contrast to other formulations such as Wilson Fermions which break all chiral symmetries or staggered Fermions which break them partially. Since the number of pions and their nature is intimately related to the actually realized chiral symmetry on the lattice, we should expect any realization of chiral Fermions on the lattice to provide insight into the question we address.

The overlap Dirac operator ($D$) can be defined [13] in terms of the Wilson-Dirac operator ($D^\dagger_w D_w$) by the relation

$$D = 1 - D^\dagger_w (D^\dagger_w D_w)^{-1/2}. \quad (1)$$

The computation of $D^{-1}$ needs a nested series of two matrix inversions for its evaluation (each step in the numerical inversion of $D$ involves the inversion of $D^\dagger_w D_w$). This squaring of effort makes a study of QCD with dynamical overlap quarks very expensive. As a first step in this direction, we chose to work with quenched overlap quarks: to study the pattern of chiral symmetry restoration and screening masses at high temperature.

We generated quenched QCD configurations at temperatures of $T/T_c = 1.25, 1.5$ and $2$ on $4 \times 8^3$ and $4 \times 12^3$ lattices (see Table I). The corresponding couplings are respectively $\beta = 5.8, 5.8941$ and $6.0625$. The configurations were separated by 1000 sweeps of a Cabibo-Marinari update. A previous computation [12] with $T = 0$ quenched overlap quarks at the nearby couplings of $\beta = 5.85$ and $6.0$ allows us to compare finite and zero temperature physics.

For the matrix $M = D^\dagger_w D_w$, and a given source vector $b$, we computed $y = M^{-1/2} b$ by a conjugate gradient (CG) version of a proposed Lanczos method [14]. CG gives better control over errors than Lanczos or other methods based on approximations using Chebychev or Reeves polynomials. In CG, the vector $x = M^{-1/2} b$ is obtained by iterating the residual vector $r_{i+1} = r_i - \alpha_i M p_i$ and the direction of change $p_{i+1} = \beta_{i+1} p_i + r_{i+1}$, where $\alpha_i = (r_{i+1}, r_i)/ (p_i, M p_i)$ and $\beta_{i+1} = (r_{i+1}, r_{i+1})/ (r_{i+1}, r_i)$. The iterations are stopped when $(r_i, r_i) < \epsilon$, for a pre-determined tolerance $\epsilon$. Let $N_s$ be the number of CG-iterations at stopping. In the orthonormal basis made of $q_i = r_i/(r_i, r_i)^{1/2}$, the matrix $M$ can be approximated by $Q^\dagger T Q$, where $Q$ is made from the set $\{ q_i \}$ and $T$ is a tridiagonal symmetric matrix of dimension $N_s$. The non-zero elements of $T$ are $T_{i,i} = 1/\alpha_i + \beta_i/\alpha_{i-1}$ and
\[ T_{i+1} = -\sqrt{\beta_i} / \alpha_{i-1}. \]
Denoting by \( \Lambda \) the diagonal matrix of the eigenvalues of \( T \), and by \( U \) its diagonalizer made from the corresponding eigenvectors, the desired solution is \( y = M^{-1/2} b \approx Q^\dagger U \Lambda^{-1/2} U Q b \), when the CG iterations are started with \( r_0 = p_0 = b \).

![Graph](image.png)

**FIG. 1.** Projection on the \( xy \) plane of two typical eigenvectors on a \( 4 \times 12^3 \) lattice at \( T = 1.5 T_c \). The zero eigenvector (top) is strongly localized while the non-zero eigenvector (bottom) is not.

A massive overlap operator is defined by
\[
D(ma) = ma + (1 - ma/2) D, \tag{2}
\]
where \( m \) is the bare quark mass, \( a \) the lattice spacing, and \( D \) is defined in [1]. We used the usual quark propagator, \( G(ma) = [1 - D/2] D^{-1}(ma) \) [14]. We computed \( G \) on 12 point sources (3 colors and 4 spins) for 10 quark masses from \( ma = 0.001 \) to 0.5 using a multiform inversion of \( D^3 D \). The (negative) Wilson mass term in \( D, \) \( (2) \) was made on each configuration with a Lanczos method in each chiral sector. Whenever \( \mu^2 \simeq O(10^{-5}) \) was obtained, the few lowest eigenvalues and eigenvectors were refined to a precision of about \( 10^{-8} \) by a Ritz functional minimization.

For each configuration we verified that the Ginsparg-Wilson [1] relation is satisfied to an accuracy of \( 10^{-9} \), thus ensuring a very precise implementation of chiral symmetry for our simulations. Another test of the precision of our measurements was provided by a check of the chiral Ward identity—
\[
a^2 \chi_{PS} = \frac{1}{ma} a^3 \langle \bar{\psi} \psi \rangle, \tag{3}
\]
where \( \langle \bar{\psi} \psi \rangle \) is the chiral condensate and \( \chi_{PS} \) is the pseudoscalar susceptibility [13]. In all our computations we found that the equality was satisfied to better than 1 part in \( 10^3 \).

For most configurations we found that the spectrum of \( D^1 D \) starts well away from zero. However, for some configurations we found zero and near-zero modes with \( \mu^2 \lt 10^{-4} \) clearly separated by a gap from the non-zero modes with \( 0.1 \lt \mu^2 \lt 10^{-3} \). The non-zero modes clearly came in degenerate pairs of opposite chiralities. For \( T = 1.5 T_c \) and \( 2 T_c \) the zero modes were all less than \( 10^{-7} \) and of definite chirality. Their numbers decreased rapidly with either increasing \( T \) or decreasing lattice size (see Table I for details). We constructed a gauge-invariant measure of localization [20] for a normalized eigenvector \( \Phi(i) \) where \( i \) stands for position, spin, and color, as the following sum,
\[
\sigma = \sum_{\text{sites}} \left[ \sum_{\text{spin, color}} \mathcal{P}(i) \Phi(i) \right]^2. \tag{4}
\]
This varies from unity for an eigenmode localized at just one site to \( 1/V \) for an eigenmode spread uniformly on a lattice of volume \( V \). On \( 4 \times 12^3 \) lattices we found \( \sigma \approx (3 - 8) \times 10^{-3} \) for the zero modes and \( \sigma \leq 10^{-3} \) for the non-zero modes (see Figure I). At \( T = 1.25 T_c \) we also found near-zero modes with \( \mu^2 \lt 10^{-4} \). These were as localized as the zero modes, but came paired in parity like the non-zero modes.

The zero modes of chiral Fermions are related to instanton-like configurations [21]. These are, in turn, known to break axial \( U(1) \) symmetry. For two flavors, the order parameter for the axial \( U(1) \) symmetry [24] is the difference of the flavor singlet and triplet scalar susceptibilities—
\[
\omega = \chi_S^3 - \chi_S^0 = \frac{4}{m^2} \langle (n_+ - n_-)^2 \rangle / V, \tag{5}
\]
where \( n_+ \) and \( n_- \) are the number of eigenvalues of \( D \) with left and right handed chiralities, and the difference needs to be evaluated only for the zero modes. In the quenched theory \( \omega \), if non-zero, is singular in the \( m \to 0 \) limit since \( \langle (n_+ - n_-)^2 \rangle \) is independent of \( m \). This is related to well known problems with \( \chi_S^0 \) in the quenched theory [23]. Combining our data with [24] we find some evidence that \( \langle (n_+ - n_-)^2 \rangle / V \) falls as a high power of \( T/T_c \). Nevertheless in quenched QCD, \( U(1) \) symmetry is not completely restored even at \( 2 T_c \).

Our measurement of \( \langle \bar{\psi} \psi \rangle \) comes from the diagonal part of \( G(ma) \) on the 12 sources used for each configuration. The analysis proceeds by writing \( G \) in terms of the eigenvectors \( \Phi_\alpha \) of \( D^1 D \) with eigenvalue \( \mu^2 \) and chirality \( \alpha \),
\[
G_{ij} = \sum_{\alpha} \frac{\Phi_\alpha(i) \Phi_\alpha(j)}{\mu^2 + (ma)^2 \lambda^2}, \tag{6}
\]
where \( \lambda^2 = 1 - \mu^2 / 4 \). The contribution of a zero mode can be easily read off from the equation above and is seen to be proportional to \( \Phi \bar{\Phi} \) and \( 1/ma \). Since the eigenvector
corresponding to the zero mode is localized, its contribution to the condensate depends strongly on the spatial position of the source vector. The remaining modes are delocalized and closely spaced; so the overlap of the eigenvector on the source is averaged out.

Our precise determination of the eigenvectors and eigenvalues allows us to subtract out the zero mode contributions in (6), although it can sometimes be a couple of orders of magnitude larger than the remainder. The subtracted condensate is strikingly identical to that seen in the sample without zero modes, at all the couplings and lattice sizes studied. We found that $\langle \psi \psi \rangle$ varies linearly with $ma$ and goes to zero as $ma \to 0$. This is how chiral symmetry restoration manifests itself in quenched QCD.

In the thermodynamic and continuum limits, it is not clear whether the near-zero modes are related to chiral symmetry breaking; on any finite $V$ they are not, but in these limits they may accumulate at zero. If they do, then $\langle \psi \psi \rangle$ would not go to zero with $m$ even above $T_c$ in the quenched theory. Clearly, one needs to examine these limits very carefully. At $T = 1.25T_c$ the number of near-zero modes is insignificant, but it seems that for $T < 1.25T_c$ their numbers will be larger [24] and the $m \to 0$ limit will have to be taken after the $V \to \infty$ limit. Quite likely, such a limit may have to be taken at more than one lattice spacing.

For lattice Fermions which satisfy the Ginsparg-Wilson relation [17], the following identities hold in the chirally symmetric phase as $ma \to 0$,

$$CS(z) = -C_{PS}(z) \quad \text{and} \quad CV(z) = C_{AV}(z). \quad (7)$$

Here $C$ is the screening correlation function in the spatial $z$ direction of an operator summed in the other three directions. The subscripts $PS$ refer to a pseudo-scalar operator, $S$ to a scalar, $V$ to a vector and $AV$ to an axial-vector [25]. We find that the $V$ and $AV$ correlators indeed agree at all $z$ and at all temperatures we studied. This is in agreement with our conclusion that the temperature range we studied has chiral symmetry.

It is clear from the chiral Ward identity [3] that large fluctuations in $\langle \psi \psi \rangle$ due to the zero mode must also lead to similar non-statistical fluctuations in $C_{PS}$. Further, since a zero mode contributes identically to $C_S$ and $C_{PS}$, the two can even have the same sign if this contribution is large enough [24]. Ignoring the configurations with zero modes, the $S$ and $PS$ correlators do obey the identity in (6), suggesting that simple results could be seen by eliminating the zero mode contribution.

One way to do this is to use the measured $\Phi$’s to subtract the zero modes and construct a new correlator $C_{PS}(z)$. Alternatively, we could consider the difference, $(C_S(z) - C_{PS}(z))/2$, which should equal $\overline{C}_{PS}(z)$. Figure 3 exhibits the comparison of the three correlators. Similar excellent agreement is also seen for these correlators for all $ma < 0.1$ and at other $T$.

After subtracting the effects of the zero mode, we find that the correlator identities are satisfied for the $S/PS$ sector as well as $V/AV$. In addition, $C_V$ is described well by an ideal gas of overlap quarks on the same lattice, as illustrated in Figure 2 (although the figure shows this only for one quark mass and $T$, this is true for all $T \geq 1.25 T_c$ and all $ma < 0.1$). While $C_{PS}$ seems to differ from the ideal gas result, the measured values of the $PS$ screening masses, $M_{PS}$, are only 10% smaller than ideal gas screening masses. This difference is small enough to be plausibly explained in a weak-coupling computation, quite unlike earlier results from staggered or Wilson quarks.

Differences between $T = 0$ mesons and our measurements are extremely clear. For $T \geq 1.25 T_c$, $M_{PS}$ is constant and non-vanishing for $ma \lesssim 0.1$. In the same temperature range, the ratio $m_{PS}(T)/m_V(T)$ is within 10% of unity and quite different from the measured values at $T = 0$ at nearby couplings $\beta$ [15]. Thus, the simple picture that emerges is a property of the high temperature phase of (quenched) QCD.
In conclusion, working with chiral (overlap) Fermions, we have found several new results and a consistent picture of the high temperature phase of quenched QCD. Axial $U(1)_{A}$ symmetry is not restored even at $2T_c$. As a result the thermal ensemble contains gauge fields which give rise to Fermion zero modes of definite chirality. When the effect of these modes is subtracted, $\langle \bar{\psi}\psi \rangle$ vanishes in the zero quark mass limit, showing that chiral symmetry is restored. Simultaneously, parity doubling is seen in the spectrum of screening masses, which are close to those expected in an ideal Fermi gas, even for the S/PS sector. Since some of these results are not obtained with staggered quarks, it is an interesting question whether the two flavor QCD phase transition is properly described by such a representation of quarks.

Some interesting problems remain to be solved. At $T \leq 1.25T_c$, there are near-zero modes. It cannot be ruled out that these modes shift the quenched chiral symmetry restoration point away from $T_c$. However, this question is crucially related to the evolution of near-zero modes with lattice volume and spacing. Hence the nature of these complications, and the question of whether they are quenched artifacts or remain in full QCD, will only become clear with further studies which are underway.

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![FIG. 4. The screening correlators on 4.12³ lattices at $T = 1.5T_c$ for $ma = 0.001$, in analyses without zero modes. The $V/AV$ correlators (boxes) agree very well with the ideal gas computation (solid line), and the $S/PS$ correlators (circles) are also similar.](image)

| $T/T_c$ | $V$ | $N_c$ | $N_0$ | $N_0'$ | $\langle \bar{\psi}\psi \rangle/(mT^2)$ | $M_{PS}/T$ | $M_{V}/T$ |
|---------|-----|-------|-------|-------|-----------------|-----------|-----------|
| 1.25    | $4 \times 10^3$ | 50    | 18    | 4     | 13.24 (9)       | 6.0 (2)   | 6.6 (1)   |
| 1.50    | $4 \times 10^3$ | 50    | 8     | 0     | 13.31 (8)       | 6.0 (1)   | 6.5 (1)   |
| 2.00    | $4 \times 10^3$ | 50    | 1     | 0     | 13.34 (6)       | 6.0 (1)   | 6.5 (1)   |
| 1.50    | $4 \times 10^4$ | 100   | 1     | 0     | 13.36 (5)       | 6.0 (2)   | 6.5 (2)   |
| 2.00    | $4 \times 10^4$ | 26    | 0     | 0     | 13.34 (8)       | 6.0 (1)   | 6.5 (1)   |

**TABLE I.** Temperatures ($T$), the lattice volume ($V$), and the number of configurations analysed ($N_c$). Also shown are the number of zero modes ($N_0$) and near-zero modes ($N_0'$), and $\langle \bar{\psi}\psi \rangle/m$, and the PS and V screening masses for $m \to 0$.  

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