The QCD phase transition with physical-mass, chiral quarks
(HotQCD Collaboration)

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We report on the first lattice calculation of the QCD phase transition using chiral fermions at physical values of the quark masses. This calculation uses 2+1 quark flavors, spatial volumes between (4 fm)3 and (11 fm)3 and temperatures between 139 and 196 MeV. Each temperature was calculated using a single lattice spacing corresponding to a temporal Euclidean extent of NT = 8. The disconnected chiral susceptibility, χdisc shows a pronounced peak whose position and height depend sensitively on the quark mass. We find no metastability in the region of the peak and a peak height which does not change when a 5 fm spatial extent is increased to 10 fm. Each result is strong evidence that the QCD “phase transition” is not first order but a continuous cross-over for mp = 135 MeV. The peak location determines a pseudo-critical temperature Tc = 155(1)(8) MeV. Chiral SU(2)L × SU(2)R symmetry is fully restored above 164 MeV, but anomalous U(1)A symmetry breaking is non-zero above Tc and vanishes as T is increased to 196 MeV.

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As the temperature of the QCD vacuum is increased above the QCD energy scale ΛQCD = 300 MeV, asymptotic freedom implies that the vacuum breaking of chiral symmetry must disappear and the familiar chirally-asymmetric world of massive nucleons and light pseudo-Goldstone bosons must be replaced by an SU(2)L × SU(2)R symmetric plasma of nearly massless up and down quarks and gluons. Predicting, observing and characterizing this transition has been an experimental and theoretical goal since the 1980’s. General principles are consistent with this being either a first-order transition for sufficiently light pion mass or a second-order transition in the O(4) universality class at zero pion mass with cross-over behavior for non-zero mp. While second order behavior is commonly expected, first-order behavior may be more likely if anomalous U(1)A symmetry is partially restored at Tc resulting in an effective U3L(2) × U3R(2) symmetry [1, 2].

The importance of the SU(2)L × SU(2)R chiral symmetry of QCD for the phase transition has motivated the widespread use of staggered fermions in lattice studies of QCD thermodynamics because this formulation possesses one exact chiral symmetry at finite lattice spacing, broken only by the quark mass. However, the flavor symmetry of the staggered fermion formulation is complicated showing an SU4L × SU4R “taste” symmetry that is broken by lattice artifacts and made to resemble the physical SU(2)L × SU(2)R symmetry by taking the square root of the Dirac determinant, a procedure believed to have a correct but subtle continuum limit for non-zero quark masses.
Because of these limitations, it is important to study these phenomena using a different fermion formulation, ideally one which supports the full $SU(2)_L \times SU(2)_R$ chiral symmetry of QCD at finite lattice spacing. It is such a study which we report here. We use Möbius domain wall fermions [3], a formulation in which the fermions are defined on a five-dimensional lattice. The extent in the fifth dimension, $L_s = 16$ or 24, making the calculation at least 16 to 24 times more costly. However, the resulting theory possesses an accurate $SU(2)_L \times SU(2)_R$ symmetry, broken only by the input quark mass and the highly suppressed mixing between the left and right four-dimensional boundaries, where the low-energy fermions propagate. This residual chiral asymmetry is a short-distance phenomenon whose leading long-distance effect is to add a constant $m_a$ to each input quark mass, $m_q$, giving a total mass $m_q = m_q + m_a$. Here the residual mass $m_a \approx 3$ MeV. Additional residual chiral symmetry breaking is $O(a^2)$ smaller [4].

Because of the computational cost of this formulation, the calculation reported here uses only one lattice spacing, $a$, at each temperature, corresponding to a single temporal extent of $N_t = 8$. The good agreement with experiment for $f_\pi$ and $f_K$ computed at our largest lattice spacing and a comparison of zero temperature results at our $T \approx 170$ lattice spacing with results from two smaller lattice spacings [3], suggest discretization errors of $\approx 5\%$ in our results. In contrast, the less costly staggered fermion calculations are performed using $N_t = 8, 10, 12$ and 16. However, to make a controlled continuum extrapolation, the staggered fermion discretization errors are assumed to behave as $a^2$. Potential non-linearities in the taste-breaking effects, which in zero-temperature staggered fermion calculations are handled using staggered chiral perturbation theory, are ignored because of the absence of a corresponding theory of finite-temperature taste breaking.

**METHODS**

The present calculation with $m_\pi = 135$ MeV and $32^3 \times 8$ and $64^3 \times 8$ volumes extends earlier domain wall fermion results with $m_\pi = 200$ MeV and $16^3 \times 8, 24^3 \times 8$ and $32^3 \times 8$ volumes [6, 7]. We use the same combination of the Iwasaki gauge action and dislocation suppressing determinant ratio (DSDR) exploited to reduce residual chiral symmetry breaking in these earlier studies. However, to enable calculations at $m_\pi = 135$ MeV with available computing resources we have changed the Shamir domain wall formulation to Möbius [3]. By choosing the Möbius parameters $b$ and $c$ of Ref. [3] so that $b - c = 1$, we insure that our Möbius Green’s functions will agree at the 0.1% level with those of Shamir evaluated at a much larger $L_s$. Thus, our $m_\pi = 200$ and $135$ MeV calculations are equivalent, including all lattice artifacts, except for the intended reduction in quark mass.

**TABLE I.** A summary of the $m_\pi = 135$ MeV ensembles. The units are MeV for the temperature $T$ and $10^{-5}/a$ for the masses $m_\pi$, $m_q$ and $m_a$. $N_t$, $N_{\text{tot}}$ and $N_s$ label the number of independent streams, the total equilibrated time units and the number of sites in each spatial direction, respectively.

| $T$ | $\beta$ | $N_t$ | $L_s$ | $c$ | $m_\pi$ | $m_q$ | $m_a$ | $N_{\text{tot}}$ | $N_s$ |
|-----|---------|-------|-------|-----|--------|------|-----|-----------------|-----|
| 159 | 1.633   | 32    | 24    | 1.5 | 22     | 219  | 1    | 5768            | 1   |
| 149 | 1.671   | 32    | 16    | 1.5 | 34     | 175  | 1    | 7823            | 1   |
| 154 | 1.689   | 32    | 16    | 1.5 | 75     | 5376 | 120  | 6108            | 4   |
| 159 | 1.707   | 32    | 16    | 1.5 | 112    | 5230 | 91   | 8714            | 3   |
| 164 | 1.725   | 32    | 16    | 1.5 | 120    | 5045 | 68   | 7149            | 4   |
| 168 | 1.740   | 32    | 16    | 1.2 | 126    | 4907 | 57   | 5840            | 2   |
| 177 | 1.771   | 32    | 16    | 1.0 | 132    | 4614 | 43   | 8467            | 2   |
| 186 | 1.801   | 32    | 16    | 1.0 | 133    | 4345 | 26   | 10127           | 2   |
| 195 | 1.829   | 32    | 16    | 0.9 | 131    | 4122 | 19   | 10124           | 2   |

Table II lists the parameters for the $m_\pi = 135$ MeV ensembles and the measured values for the residual mass. At the lowest temperatures, more than 90% of the quark mass is generated by residual chiral symmetry breaking. In addi-
TABLE II. Results at $\beta = 1.633$ and $T = 0$ (in lattice units and MeV) from 25 configurations separated by at least 20 time units. We use $M_0$ to fix the scale. Also listed are the experimental values.

| $m_\pi$ | MeV | Expt.(MeV) |
|---|---|---|
| 0.1181(5) | 129.2(5) | 135 |
| 0.4203(5) | 462.5(5) | 495 |
| 1.530(3) | 1672.45 | 1672.45 |
| $T = \frac{1}{8\alpha}$ | 0.125 | 136.7(3) |
| $f_\pi$ | 0.1263(2) | 138.1(2) | 130.4 |
| $f_K$ | 0.1483(4) | 162.2(4) | 156.1 |
| $m_{\pi\text{exp}}$ | 0.00217(2) | — | — |

RESULTS

Our most dramatic result is the temperature-dependent, disconnected chiral susceptibility $\chi_{\text{disc}}$, plotted in Fig. 1. Three of the four lower curves show earlier results with $m_\pi = 200$ MeV on $16^3$, $24^3$ and $32^3$ volumes. A significant decrease in $\chi_{\text{disc}}$ is seen for temperatures below 165 MeV as the volume is increased above $16^3$, a volume dependence anticipated in earlier scaling [8, 9] and model [10] studies. The two higher curves show a large increase in $\chi_{\text{disc}}$ in the entire transition region for $m_\pi = 135$ MeV and both $32^3$ and $64^3$ volumes. The ratio of peak heights for the $m_\pi = 135$ and 200 MeV, $32^3$ data is 2.1(0.2), which is consistent with the ratio 1.86 predicted by universal $O(4)$ scaling $\sim m_\pi^{1/\delta-1} \propto m_\pi^{-1.5854}$, only if the regular, mass-independent part of $\chi_{\text{disc}}$ is small.

This comparison of $\chi_{\text{disc}}$ with universal $O(4)$ scaling neglects the connected part of the chiral susceptibility. We find that the connected chiral susceptibility has a mild dependence on both the temperature and quark mass (as is expected if the $\delta$ screening mass remains non-zero at $T_c$) and so does not contribute to the singular part of the chiral susceptibility.

Also shown in this figure are HISQ results for $N_t = 12$ and a Goldstone pion mass of 161 MeV [8, 11]. If scaled to $m_\pi = 135$ MeV assuming this same $m_\pi^{-1.5854}$ behavior, the HISQ value for $\chi_{\text{disc}}$ is 50% smaller than that seen here. This discrepancy reaffirms the importance of an independent study of the order of the transition and calculation of $T_c$ using chiral quarks.
The peak shown in Fig. 1 implies a pseudo-critical temperature of 155(1)(8) MeV. The central value and statistical error are obtained by fitting the $T = 149, 154$ and 159 MeV values of $\chi_{\text{disc}}$ to a parabola. The second, systematic error reflects the expected 5% discretization error. We do not include a systematic error caused by our finite volume. While typically neglected when $N_\sigma/N_t \geq 4$, we lack the data needed for an empirical estimate. This result for $T_c$ is consistent with the continuum limit for this quantity obtained using staggered fermions [11, 12].

The order of the QCD phase transition can now be studied using the time-history of the chiral condensate for $T \approx T_c$. Figure 2 shows four time histories of $\langle \bar{q} q \rangle$ at $T = 154$ MeV. All four streams fluctuate over the same range of values, showing no metastable behavior and no difference between those streams starting from ordered versus disorder configurations. This and the failure of $\chi_{\text{disc}}$ to grow as $2^3$ when the volume is increased from $32^3$ to $64^3$ provide strong evidence that for $m_\sigma = 135$ MeV, the QCD phase transition is not first-order but a crossover, a conclusion consistent with previous staggered work [11, 12].

In Fig. 3 we show the $SU(2)_L \times SU(2)_R$-breaking differences between the susceptibilities $\chi_\pi$ and $\chi_\sigma$ and between $\chi_\delta$ and $\chi_\eta$. Each pair of fields, $(\bar{\pi}, \sigma)$ and $(\bar{\delta}, \eta)$ forms a 4-dimensional representation of $SU(2)_L \times SU(2)_R$ symmetry. These $SU(2)_L \times SU(2)_R$-breaking differences are large below $T_c$ but have become zero for $T > 168$ MeV.
\( T > 164 \text{ MeV} \). In Fig. 4 we show the difference \( \chi_\pi - \chi_\delta \). This pair of quantities is related by the anomalous \( U(1)_A \) transformation, a symmetry of the classical field theory that is broken by the axial anomaly. Figure 4 shows that this symmetry is not restored until at least \( T \geq 196 \text{ MeV} \). Also shown in this figure is the result from our earlier \( m_\pi = 200 \text{ MeV} \) calculation [7]. The expected increase in \( \chi_\pi - \chi_\delta \) with decreasing pion mass is seen for \( T \leq T_c \). However, above \( T = 168 \text{ MeV} \) this difference is still non-zero and has become mass independent, confirming our previous conclusion that this non-zero value is a result of the axial anomaly, not the small quark mass.

\section*{CONCLUSION}

We have presented results from the first study of the QCD phase transition using chirally symmetric lattice fermions, physical quark masses and therefore three degenerate pions with \( m_\pi \approx 135 \text{ MeV} \). We find \( T_c = 155(1)(8) \text{ MeV} \), similar to previous staggered fermion results, and see cross-over behavior, consistent with a second order critical point at zero quark mass. We show that anomalous symmetry breaking extends to temperatures approximately 30 MeV above \( T_c \). Finally, we see a factor of two increase in the disconnected chiral susceptibility, \( \chi_{\text{disc}} \) near \( T_c \) as \( m_\pi \) decreases from 200 to 135 MeV, similar to the expectations for critical \( O(4) \) scaling, provided the regular part of \( \chi_{\text{disc}} \) is small. However, in this region we find \( \chi_{\text{disc}} \) 50\% larger than that suggested by staggered fermion results.

These results may close a chapter in the study of the QCD phase transition. The cross-over character and pseudo-critical temperature of the transition have now been obtained using a formulation which respects the symmetries of QCD, uses physical values for both the strange and light quark masses and is performed for values of the inverse lattice spacing \( 1/a \geq 1.1 \text{ GeV} \) where 5\% discretization errors are to be expected. This is a challenging calculation with 5-dimensional lattice volumes as large as \( 64^3 \times 8 \times 24 \) and a physically light quark mass. This study was made possible by the use of the DSDR action [16], Möbius fermions [3], highly efficient code [17] and substantial resources provided by the Lawrence Livermore National Laboratory. Of course, it remains important to continue to explore these questions at larger spatial volume and smaller lattice spacing when adequate resources become available.

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