Chiral Phase Transition Temperature in (2 + 1)-Flavor QCD

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We present a lattice-QCD-based determination of the chiral phase transition temperature in QCD with two degenerate, massless quarks and a physical strange quark mass using lattice QCD calculations with the highly improved staggered quarks action. We propose and calculate two novel estimators for the chiral transition temperature for several values of the light quark masses, corresponding to Goldstone pion masses in the range of 58 MeV ≤ mφ ≤ 163 MeV. The chiral phase transition temperature is determined by extrapolating to vanishing pion mass using universal scaling analysis. Finite-volume effects are controlled by extrapolating to the thermodynamic limit using spatial lattice extents in the range of 2.8–4.5 times the inverse of the pion mass. Continuum extrapolations are carried out by using three different values of the lattice cutoff, corresponding to lattices with temporal extents Nτ = 6, 8, and 12. After thermodynamic, continuum, and chiral extrapolations, we find the chiral phase transition temperature Tc ≡ 132 ± 6 MeV.

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Introduction.—For physical values of the light up, down, and heavier strange quark masses, strongly interacting matter undergoes a transition from a low-temperature hadronic regime to a high-temperature region that is best described by quark and gluon degrees of freedom. This smooth crossover between the two asymptotic regimes is not a phase transition [1]. It is characterized by a pseudocritical temperature, Tpc, that has been determined in several numerical studies of quantum chromodynamics (QCD) [2–4]. A recent determination of Tpc extracted from the maximal fluctuations of several chiral observables gave Tpc = (156.5 ± 1.5) MeV [5].

In the chiral limit of (2 + 1)-flavor QCD, i.e., where two (degenerate) light quark masses m_i = (m_u + m_d)/2 approach zero but the strange quark mass m_s is kept fixed to its physical value, the pseudocritical behavior is expected to give rise to a “true” chiral phase transition [6,7]. The chiral phase transition temperature itself is expected to set an upper bound on the temperature at a possible critical point at nonzero baryon chemical potential [8,9], which is intensively searched for in heavy ion collision experiments. Whether this chiral phase transition is first or second order may depend crucially on the temperature dependence of the chiral anomaly [7]. In the latter case, critical behavior generally is expected to be controlled by the 3D O(4) universality class, although a larger 3D universality class [10,11] may become of relevance in case the axial anomaly also gets restored effectively at Tc. If the chiral phase transition is first order, then a second-order phase transition, belonging to the 3D Z(2) universality class, would occur for m_i > 0. When decreasing the light to strange quark mass ratio, H = m_i/m_s, towards zero, this would give rise to diverging susceptibilities already for some critical mass ratio Hc = m_i/m_s > 0. The analysis presented here leads to a determination of the critical temperature Tc0. However, as we do not have any evidence for Hc ≠ 0, we de facto present a determination of the chiral phase transition temperature Tc0.

Although Tc0 appears as a fit parameter in all finite-temperature scaling studies of the chiral transition in QCD [3,12,13], so far no lattice QCD calculation has carried out a systematic analysis of Tc0 by controlling thermodynamic, continuum, and chiral limits. Here, we will present a first

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lattice-QCD-based determination of $T_c^0$ in $(2+1)$-flavor QCD with controlled thermodynamic, continuum, and chiral extrapolations. QCD-inspired model calculations [14,15] suggest that $T_c^0$ might be even lower (by 20–30 MeV) than $T_{pc_c}$. To mitigate this potentially large $m_l$ dependence of $T_{pc}$ while approaching $m_l \to 0$, we propose two novel estimators of the pseudocritical temperature having only mild dependence on $m_l$, leading to well-controlled chiral extrapolation.

**Chiral observables.**—At low temperatures, chiral symmetry is spontaneously broken in QCD. An order parameter for the restoration of this symmetry at high temperature is the chiral condensate, which is obtained as the derivative of the partition function, $Z(T,V,m_u,m_d,m_s)$, with respect to one of the quark masses, $m_i$,

$$\langle \bar{\psi}\psi \rangle_i = \left. \frac{T \partial \ln Z(T,V,m_u,m_d,m_s)}{\partial m_i} \right|_{m_i=m}.$$  \hspace{1cm} (1)

The light quark chiral condensate, $\langle \bar{\psi}\psi \rangle_i = (\langle \bar{\psi}\psi \rangle_u + \langle \bar{\psi}\psi \rangle_d)/2$, is an order parameter for the chiral phase transition that occurs in the limit $m_l \to 0$. For nonvanishing $m_l$, this order parameter requires additive and multiplicative renormalization. We take care of this by introducing a combination of the light and strange quark chiral condensates,

$$M = 2(m_i \langle \bar{\psi}\psi \rangle_i - m_l \langle \bar{\psi}\psi \rangle_s)/f_K^2,$$  \hspace{1cm} (2)

where the kaon decay constant, $f_K = 156.1(9)/\sqrt{2}$ MeV, for physical values of the degenerate light and strange quark mass, is used as a normalization constant to define a dimensionless order parameter $M$. The order parameter $M$ is free of UV divergences linear in the quark masses $m$ [3] but may still receive divergent contributions proportional to $m^3 \ln(m)$, which we neglect here. The derivative of $M$ with respect to the light quark masses gives the chiral susceptibility,

$$\chi_M = m_i(\partial_{m_u} + \partial_{m_d})M|_{m_u=m_d} = m_i(m_s \chi_l - 2\langle \bar{\psi}\psi \rangle_s - 4m_s \chi_{ss})/f_K^2,$$ \hspace{1cm} (3)

with $\chi_{fg} = \partial_{m_g} \langle \bar{\psi}\psi \rangle_g$ and $\chi_l = 2(\chi_{uu} + \chi_{ud})$.

When approaching the chiral limit, one also needs to control the thermodynamic limit, $V \to \infty$. In the vicinity of a second-order phase transition, $M$ and $\chi_M$ are given in terms of the universal finite-size scaling functions $f_G(z,z_L)$ and $f_x(z,z_L)$, which depend on the scaling variables $z = t/h^{1/\beta}$ and $z_L = h/t_0/(Lh^{1/\beta})$. Here $t = (T - T_c^0)/(t_0 T_c^0)$ denotes the reduced temperature; $h = H/h_0$ is the symmetry-breaking field; and $L/t_0$ parametrizes the finite size of the system, $L \equiv V^{1/3}$. These scaling variables are expressed in terms of nonuniversal parameters, $t_0$, $h_0$, $t_0$.

While the universal scaling functions control the behavior of $M$ and $\chi_M$ close to a critical point at $(z,z_L) = (0,0)$, they also receive contributions from corrections to scaling and regular terms [16,17], which we represent by a function $f_{sub}(T,H,L)$. With this, we may write

$$\chi_M = h_0^{-1} h^{1/\beta - 1} f_x(z,z_L) + f_{sub}(T,H,L).$$  \hspace{1cm} (4)

As far as is needed for the analysis, we will specify contributions arising from $f_{sub}(T,H,L)$ later.

Close to the thermodynamic limit, $f_x(z,z_L)$ has a pronounced peak, which often is used to define a pseudocritical temperature $T_p$. In the scaling regime, this peak is located at some $z = z_p(z_L)$, which defines $T_p$.

$$T_p(H,L) = T_c^0 \left( 1 + \frac{z_p(z_L)^2}{z_0} H^{1/\beta} \right) + \text{subleading},$$  \hspace{1cm} (5)

with $z_0 = h_0^{1/\beta}/t_0$. While the first term describes the universal quark mass dependence of $T_p$, corrections may arise from corrections to scaling and regular terms, shifting the peak location of the chiral susceptibilities.

When approaching the chiral limit, depending on the magnitude of $z_p/z_0 \approx z_p(0)/z_0$, $T_p(H,L)$ may change significantly with $H$. In the potentially large temperature interval between $T_c^0$ and $T_p(H,L)$, regular contributions, arising from $f_{sub}(T,H,L)$, may also be large, and during the $H \to 0$ extrapolation several nonuniversal parameters may be needed to account for contributions from $f_{sub}(T,H,L)$. It is thus advantageous to determine $T_c^0$ using observables defined close to $z \approx 0$. While $T_p(H,L)$, defined through such observables for small $H > 0$, will have milder $H$ dependence, the determination of $T_c^0 = T_p(H \to 0,L \to \infty)$ will be well controlled.

We will consider here two estimators for $T_c^0$, defined at or close to $z = 0$. We determine temperatures $T_{\delta}$ and $T_{60}$ by demanding

$$H \chi_M(T_{\delta},H,L) = \frac{1}{6};$$ \hspace{1cm} (6)

$$\chi_M(T_{60},H) = 0.6 \chi_M^{\max}. \hspace{1cm} (7)$$

Equation (6) has already been introduced in Ref. [18] as a tool to analyze the chiral transition in QCD, and it is understood that $T_{60}$ is determined at a temperature on the left of the peak $\chi_M^{\max}$, i.e., $T_{60} < T_p$. These relations define pseudocritical temperatures, $T_{\delta}$, which are close to $T_c^0$ already for nonzero $H$ and $L^{-1}$. They converge to the chiral phase transition temperature $T_c^0$ in the thermodynamic and chiral limits. For nonzero $L^{-1}$, Eqs. (6) and (7) involve scaling variables $z_{\delta}(z_L)$ which approach or are close to zero in the limit $L^{-1} \to 0$, i.e., $z_{\delta} \equiv z_{\delta}(0) = 0$ and $z_{60} \equiv z_{60}(0) \approx 0$. Some values for $z_{60}$ for several universality classes, are given in Table I, and the relevant scaling functions, obtained in the thermodynamic limit $z_L = 0$, are shown in Fig. 1.
TABLE I. The critical exponent δ, the location of the peak $z_p$, and the position of 60% of the peak value $z_{60}$ of the scaling functions $f_\delta(z)$ for different 3D universality classes [17,19,20]. Also given are $f_G(z_p)$, $f_\delta(z_p)$, and $r_\delta(0) = f_\delta(0)/f_G(z_p)$.

| $\delta$ | $z_p$   | $z_{60}$ | $f_G(z_p)$ | $f_\delta(z_p)$ | $r_\delta(0)$ |
|----------|---------|----------|------------|----------------|--------------|
| $Z(2)$   | 4.805   | 2.00(5)  | 0.10(1)    | 0.548(10)      | 0.3629(1)    |
| $O(2)$   | 4.780   | 1.58(4)  | -0.005(9)  | 0.550(10)      | 0.3489(1)    |
| $O(4)$   | 4.824   | 1.37(3)  | -0.013(7)  | 0.532(10)      | 0.3430(1)    |

Ignoring possible corrections from contributions to scaling, and keeping in $f_{\text{sol}}$ only the leading $T$-independent, infinite-volume regular contribution proportional to $H$, we then find for the pseudocritical temperatures

$$T_X(H,L) = T_0^\delta \left( 1 + \left( \frac{z_X(z_L)}{z_0} \right) H^{1/\delta} \right) + c_X H^{1-1/\delta+1/\delta^2}, \quad X = \delta, 60. \quad (8)$$

The universal functions, $z_X(z_L)$, may directly be determined from the ratio of scaling functions, $f_\delta(z_\delta, z_L)/f_G(z_\delta, z_L) = 1/\delta$ and $f_\delta(z_{60}, z_L)/f_\delta(z_p, z_L) = 0.6$, respectively. The finite-size scaling functions $f_\delta(z, z_L)$ have been determined for the 3D, $O(4)$ universality class in Ref. [21].

We will present here results on $T_\delta$ and $T_{60}$ obtained in lattice QCD calculations [22]. We have calculated the chiral order parameter $M$ and the chiral susceptibility $\chi_M$ [Eqs. (2) and (3)] in $(2+1)$-flavor QCD with degenerate up and down quark masses ($m_u = m_d$). For our lattice QCD calculations, performed with the highly improved staggered quark (HISQ) action [23] in the fermion sector and the Symanzik improved gluon action, the strange quark mass has been tuned to its physical value [24], and the light quark mass has been varied in a range $m_s \in [m_s/160 : m_s/20]$ corresponding to Goldstone pion masses in the range $58 \text{ MeV} \lesssim m_\pi \lesssim 163 \text{ MeV}$. At each temperature, we performed calculations on lattices of size $N^3L$, for three different values of the lattice cutoff, $aT = 1/N_t$, with $N_t = 6, 8, 12$. In the HISQ discretization scheme, so-called taste symmetry violations give rise to a distortion of the light pseudoscalar (pion) meson masses. These discretization effects are commonly expressed in terms of a root-mean-square (rms) pion mass which approaches the Goldstone pion mass in the continuum limit. For our computational setup and the three different values of the lattice cutoff, this has been discussed in Ref. [3]. For lattice spacings corresponding to $N_t = 6, 8, 12$, one finds for physical values of the quark masses $M_{\text{rms}} = 400, 300, 200$ MeV, respectively. The spatial lattice extent, $N_s = L/a$, has been varied in the range $4 \leq N_s/N_t \leq 8$.

For each $n_t$, we analyzed the volume dependence of $M$ and $\chi_M$ in order to perform controlled infinite-volume extrapolations.

Results.—In Fig. 2 (left), we show results for $\chi_M$ on lattices with temporal extent $N_t = 8$ for five different values of the quark mass ratio, $H = m_1/m_s$, and the largest lattice available for each $H$. The increase of the peak height, $\chi_M^{\text{max}}$, with decreasing $H$ is apparent. This rise is consistent with the expected behavior, $\chi_M^{\text{max}} \sim H^{1/\delta-1} + \text{const.}$, with $\delta \approx 4.8$; however, a precise determination of $\delta$ is not yet possible with the current data.

In Fig. 2 (right), we show the volume dependence of $\chi_M$ for $H = 1/80$ on lattices with spatial extent $N_t = 8$ and for $N_s/N_t = 4, 5, 7$. Similar results have also been obtained for $N_t = 6$ and 12. We note that $\chi_M^{\text{max}}$ decreases slightly with increasing volume, contrary to what one would expect to find at or close to a first- or second-order phase transition. Our current results, thus, are consistent with a continuous phase transition at $H_c = 0$.

Using results for $\chi_M$ and $M$, we constructed the ratios $H\chi_M(M)/M$ for different lattice sizes and several values of the quark masses. This is shown in Fig. 3 (left) for the lightest quark masses used on the $N_t = 12$ lattices, $H = 1/80$. The intercepts with the horizontal line at $1/\delta$ define $T_\delta(H, L)$. For $H = 1/80$ and each of the three temporal lattice sizes, we have results for three different volumes on which we can extrapolate $T_\delta(H, L)$ to the infinite-volume limit. We performed such extrapolations using (i) the $O(4)$ ansatz given in Eq. (8), as well as (ii) an extrapolation in $1/V$. The latter is appropriate for large $L$, if the volume dependence predominantly arises from regular terms, and the former is appropriate close to or in the continuum limit, if the singular part dominates the partition function. In the former case, we use the approximation $z_\delta(z_L) \sim z_5^{7}$, which parametrizes well the finite-size dependence of $T_\delta$ in the scaling regime [21]. The resulting fits are shown in Fig. 3 (middle).

We note that results for fixed $H$ tend to approach the infinite-volume limit more rapidly than $1/V$, which is in
accordance with the behavior expected from the ratio of finite-size scaling functions. The resulting continuum limit extrapolations in $1/N_t^2$ based on data for (i) all three $N_t$ values, as well as (ii) $N_t = 8$ and 12 only, are shown as horizontal bars in this figure. An analogous analysis is performed for $H = 1/40$. Finally, we extrapolate the continuum results for $T_\delta(H, \infty)$ with $H = 1/40$ and 1/80 to the chiral limit, using Eq. (8) with $z_\delta(0) = 0$. Results obtained from these extrapolation chains, which involve either a $1/V$ or $O(4)$ ansatz for the infinite-volume extrapolation, as well as continuum limit extrapolations performed on two different datasets, lead to chiral transition temperatures $T^0_\delta$ in the range (128–135) MeV. The resulting values for $T^0_\delta$ are summarized in Fig. 4.

As the fits shown in Fig. 3 (middle) suggest that the $O(4)$ scaling ansatz is appropriate for the analysis of finite-volume effects already at nonzero values of the cutoff, we can attempt a combined analysis of all data available for different light quark masses and volumes at fixed $N_t$. This utilizes the quark mass dependence of finite-size corrections, expressed in terms of $z_\tau$, and thus it intertwines continuum and chiral limit extrapolations. Using the scaling ansatz given in Eq. (8), it also allows us to account for the contribution of a regular term in a single fit. Fits for fixed $N_t$ based on this ansatz, using data for all available lattice sizes and $H \leq 1/27$, are shown in Fig. 3 (right). For each $N_t$, the fit yields results for $T^0_\delta(H, L)$ at arbitrary $H$. Some bands for $H = 1/40$ and 1/80 are shown in the figure. As can be seen, for $H = 1/80$, these bands compare well with the fits shown in Fig. 3 (middle). For each $N_t$, an arrow shows the corresponding chiral limit result, $T^0_\delta(0, \infty)$. We extrapolated these chiral limit results to the continuum limit and estimated systematic errors again by including or leaving out data for $N_t = 6$. The resulting $T^0_\delta$ values, shown in Fig. 4, are in complete agreement with the corresponding numbers obtained by first taking the continuum limit and then taking the chiral limit. Within the current accuracy, these two limits are interchangeable.

Similarly, we analyzed results for $T^0_{60}$ on all datasets using the same analysis strategy as for $T_\delta$. As can be seen in Fig. 4, we find for each extrapolation ansatz that the resulting values for $T^0_6$ agree to within better than 1% accuracy with the corresponding values for $T_\delta$. This corroborates that the chiral susceptibilities used for this analysis reflect basic features of the $O(4)$ scaling functions.

Performing continuum extrapolations by either including or discarding results obtained on the coarsest ($N_t = 6$) lattices leads to a systematic shift of about 2–3 MeV in the estimates for $T^0_\delta$. This is reflected in the displacement of the two bands in Fig. 4, which show averages for $T^0_\delta$ obtained
with our different extrapolation Ansätze. Averaging separately over results for \(T_0\) and \(T_{60}\) obtained with both continuum extrapolation procedures and including this systematic effect, we find for the chiral phase transition temperature

\[
T_c^0 = 132^{+3}_{-6} \text{ MeV.} \tag{9}
\]

Conclusions.—Based on two novel estimators, we have determined the chiral phase transition temperature in QCD with two massless light quarks and a physical strange quark. Equation (9) gives our thermodynamic-, continuum- with two massless light quarks and a physical strange quark. Numerical calculations have been made possible through PRACE grants at CSCS, Switzerland, and at CINECA, Italy as well as grants at the Gauss Center for Supercomputing and NIC-Jülich, Germany. These grants provided access to resources on Piz Daint at CSCS and Marconi at CINECA, as well as on JUQUEEN and JUWELS at NIC. Additional calculations have been performed on GPU clusters of USQCD, at Bielefeld University, the PC\(^2\) Paderborn University, and the Nuclear Science Computing Center at Central China Normal University, Wuhan, China. Some datasets have also partly been produced at the TianHe II Supercomputing Center in Guangzhou.

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