

The order of the chiral phase transition in massless many-flavour lattice QCD

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The nature of the QCD phase transition in the chiral limit presents a challenging problem for lattice QCD. However, its study provides constraints on the phase diagram at the physical point. In this work, we investigate how the order of the chiral phase transition depends on the number of light quark flavours. To approach the lattice chiral limit, we map out and extrapolate the chiral critical surface that separates the first-order region from the crossover region in an extended parameter space, which includes the gauge coupling, the number of quark flavours, their masses, and the lattice spacing. Lattice simulations with standard staggered quarks reveal that for each $N_f < 8$, there exists a tricritical lattice spacing $a^{\text{tric}}(N_f)$, at which the chiral transition changes from first order $(a > a^{\text{tric}})$ to second order $(a < a^{\text{tric}})$. Thus, the first-order region is merely a lattice artifact and not connected to the continuum. By determining the associated temperatures $T(N_f^{\text{tric}}, a^{\text{tric}})$ at these tricritical points, we confirm the expected decrease in the critical temperature as the number of flavours increases. The obtained temperatures define a tricritical line which is connected to the continuum and terminates at a physical $N_f^{\text{tric}}(a = 0)$. Our data is compatible with a vanishing temperature at that point, $T(N_f^{\text{tric}}(a = 0)) = 0$.

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Figure 1: Columbia plots. Every point represents a phase boundary with an implicitly associated (pseudo-) critical temperature T_c . Figures are taken from [6].

1. Introduction

The chiral limit refers to QCD in the presence of massless quarks. As a controllable deformation of QCD, it offers valuable insights into fundamental principles of the strong interaction and provides relevant constraints for physical QCD. Particularly with the aim of improving our understanding of the chiral phase transition, it is worth studying the massless limit of quarks. Only in the presence of massless quarks, the chiral symmetry is exact and thus its spontaneous breaking has to be accompanied by a true non-analytic phase transition.

How the chiral transition is affected by a change of the quark masses is illustrated in a so-called Columbia plot. Figure 1a depicts the nature of the QCD thermal transition as a function of degenerate up- and down-quark masses and the strange-quark mass [1]. The variation of masses can be used as an interpolation of QCD between one to three flavours. The chiral transition at the physical point is known to be an analytic crossover [2]. Quenched QCD in the limit of infinitely heavy masses (upper right corner) reduces to a SU(3) Yang-Mills theory in the presence of static quarks and exhibits a first-order phase transition of the \mathbb{Z}_3 -center symmetry [3–5]. However, the situation in the chiral limit (lower and upper left corner) is more delicate. Massless quarks cannot be simulated directly with Monte-Carlo simulations due to zero modes in the dirac operator. Non-perturbative statements from first principles are therefore not straightforward. Nevertheless, an increased interest in recent years has led to accumulating confirmations that QCD with both, two and three flavours, exhibit a second-order transition for massless quarks. Support for this conclusion comes from lattice methods [6–12], as well as functional approaches [13–17].

The question remains whether a second-order transition persists in the chiral limit for high numbers of flavours. This is illustrated in Fig. 1b. Instead of using the strange mass as interpolation between two and three flavours, we consider degenerate quark masses and treat the number of fermions, N_f , as a continuous real parameter. Assuming now that a first-order transition emerges at some higher number of flavours, the chiral limit features triple points characterized by the coexistence of three





(a) Szenario 1: 2nd-order transition for all N_f

(b) Szenario 2: 1st-order transition for higher N_f

Figure 2: Comparison of phase diagrams for possible scenarios for the chiral limit depending on whether a first-order transition emerges for higher N_f or not. Figures are taken from [6].

distinct states (a vanishing, positive and negative chiral condensate at the critical temperature). The onset of the triple line is marked by a tricritical point. For a detailed description see [6]. All flavours below N_f^{tric} exhibit a second-order phase transition in the chiral limit, whereas those above undergo a first-order transition. The first-order region, which also extends to non-vanishing masses, is then bounded by a \mathbb{Z}_2 -boundary line. In fact, such a \mathbb{Z}_2 -line was found by our group in lattice simulations [6, 18]. However, it was simultaneously shown that the size of the first-order region decreases with decreasing lattice spacing. It was concluded that the first-order region is thus a cutoff effect, and the transition is second-order in the continuum limit for at least $N_f \leq 6$.

In this work we extend the Columbia plot (Fig. 1b) into a phase diagram, see Fig. 2, by determining the critical temperatures. Of particular interest is the temperature at the tricritical point N_f^{tric} . A rough outline of the expected behavior of the critical temperature as a function of the number of flavours in the chiral limit can be derived from perturbation theory. For small N_f a linear decrease in *T* is predicted [19], which transitions to exponential Miransky-scaling for higher N_f [20] and ultimately ends at the onset of the conformal window. The latter arises due to the emergence of non-trivial infrared (Banks-Zaks) fixed points [21]. The perturbative two-loop beta function of the running coupling suggests the fixed points to emerge between $N_f \approx 8.05$ and 16.5. However, non-perturbative dynamics might alter the onset N_f^* of the conformal window, leaving it an open question for ongoing research. Studies suggest $8 \leq N_f^* \leq 12$ [19, 22–29], with a growing tendency towards $N_f^* = 8$ being the sill of the conformal window [30, 31]. The absence of a running coupling renders QCD scale-invariant, resulting in a chirally symmetric phase and the lack of a thermal phase transition, i.e., T = 0.

Figure 2 illustrates this expected decrease of the critical temperature with the number of flavours. Fig. 2a corresponds to the scenario that the second-order transition, found for $N_f = 2$ and 3, extends all the way down to T = 0, whereas Fig. 2b shows the potential opening of a first-order area, that is, the second-order line terminates at a finite T at N_f^{tric} and is followed by a first-order transition up to the conformal window. Both scenarios have a tricritical point N_f^{tric} but can be distinguished by its associated temperature at that point. While in scenario Fig. 2a, the tricritical point coincides with the onset of the conformal window N_f^* and has $T(N_f^{\text{tric}}) = 0$, the temperature at N_f^{tric} in scenario Fig. 2b is $T(N_f^{\text{tric}}) > 0$.

Our goal is to determine N_f^{tric} and its corresponding temperature. Once $T(N_f^{\text{tric}})$ is known, it will reveal whether the conformal window is approached through a first-order or second-order transition. In case of the latter, our approach might even pinpoint the onset of the conformal window.

2. Methodology and computational framework

Strategy

Since the chiral limit is not accessible to lattice simulations, it relies on extrapolations. If a first-order region is to emerge at higher N_f in the chiral limit, a tricritical point is guaranteed to exist which is approached by a second-order wingline with known scaling [32]

$$N_f^c(m) = N_f^{\text{tric}} + A \cdot m^{2/5} + B \cdot m^{4/5} + O(m^{6/5}).$$
(1)

Once the critical masses on this \mathbb{Z}_2 -boundary line are determined for several N_f , the tricritical point N_f^{tric} can be found by extrapolation. Nevertheless, as all simulations are performed on the lattice, the Columbia plots gets extended in another dimension consisting of the lattice spacing. In [6] it was found that the \mathbb{Z}_2 -boundary highly depends on the lattice spacing. We thus repeat mapping out the \mathbb{Z}_2 -line and extracting N_f^{tric} for several lattice spacings.

Simulation details

Our QCD lattice simulations employ the standard Wilson gauge action and unimproved staggered fermions on lattices with size $N_{\tau} \times N_{\sigma}^3$. The tuneable bare parameters are the degenerate quark mass *am*, the inverse gauge coupling $\beta = 6/g^2$ and the number of fermions N_f . The coupling β controls the lattice spacing *a* and tunes the temperature through the relation $T = 1/[a(\beta)N_{\tau}]$. By keeping *T* constant, the lattice spacing can be reduced by increasing N_{τ} . Our codebase is built on the OpenCL-based lattice QCD framework CL2QCD [33]. It is executed on the GPU clusters VIRGO at GSI in Darmstadt and Goethe-HLR at the Center for Scientific Computing in Frankfurt.

Determining the critical surface

A critical point on the \mathbb{Z}_2 -boundary corresponds to a set of critical couplings $\{\beta_c^{\mathbb{Z}_2}, am_c^{\mathbb{Z}_2}\}$ at fixed N_f and N_{τ} . The order of the chiral transitions is studied by the use of the chiral condensate as a (quasi-)order parameter, $\langle O \rangle = \langle \bar{\Psi} \Psi \rangle$, and its distribution is analysed via its generalised moments

$$B_n = \frac{\langle (O - \langle O \rangle)^n \rangle}{\langle (O - \langle O \rangle)^2 \rangle^{n/2}}.$$
(2)

To obtain the critical coupling $\beta_c^{\mathbb{Z}_2}$ and critical mass $am_c^{\mathbb{Z}_2}$ at some fixed N_f and N_τ , we perform a finite size scaling analysis. We start to determine the (pseudo-)critical β_{pc} at three different masses in the vicinity of the critical mass value $am_c^{\mathbb{Z}_2}$ by scanning in the lattice gauge coupling for vanishing skewness, $B_3(\beta_{pc}, am, N_\sigma) = 0$. This is repeated for three different aspect ratios $N_\sigma/N_\tau \in \{2, 3, 4\}$. Identifying the kurtosis $B_4(\beta_{pc}, am, N_\sigma)$ on this pseudocritical hypersurface and assuming its associated critical value of $B_4^{\mathbb{Z}_2} = 1.6044(10)$, the \mathbb{Z}_2 -critical mass is extracted by a finite size scaling fit

$$B_4(\beta_{pc}, am, N_{\sigma}) \approx \left(B_4^{\mathbb{Z}_2} + c[am - am_c^{\mathbb{Z}_2}] N_{\sigma}^{1/\nu} \right) \left(1 + b N_{\sigma}^{y_t - y_h} \right).$$
(3)

The last factor is a finite volume correction term, where $y_t = 1/v = 1.5870(10)$ and $y_h = 2.4818(3)$ are the associated 3D Ising exponents [34, 35]. Once the critical mass $am_c^{\mathbb{Z}_2}$ is known, the critical values of the coupling constant $\beta_c^{\mathbb{Z}_2}$ at $am_c^{\mathbb{Z}_2}$ are obtained by a linear fit of the (pseudo-)critical β_{pc} values at the simulated quark masses.

3. Results

3.1 Phase boundary in the lattice parameter space

The chiral critical surface that separates the first-order region from the crossover has been mapped out in an enlarged parameter space of our lattice action $\{\beta, am, N_f, N_\tau\}$. For several numbers of flavours $N_f \in [2, 8]$ and lattice spacings $N_\tau \in \{4, 6, 8, 10\}$ the critical couplings $\{\beta_c^{\mathbb{Z}_2}, am_c^{\mathbb{Z}_2}\}$ were identified, characterizing the \mathbb{Z}_2 -boundary line. Figure 3a shows the critical masses $am_c^{\mathbb{Z}_2}$ over the number of flavours; the values of the critical coupling are implicit. This figure is the lattice version of Fig. 1b and illustrates how the first-order region behaves with the lattice spacing N_τ . The indicated lines correspond to the \mathbb{Z}_2 -boundary fitted according to Eq.(1). It can be seen that the first-order region – masses below the respective lines – is highly cutoff dependent and shrinks for decreasing lattice spacing. Furthermore, the onset of the first-order region $N_f^{\text{tric}}(N_\tau)$ is pushed to higher N_f , the lower the lattice spacing. This analysis eventually raises the question, whether a first-order region even remains for any number of flavours in the continuum. This is tested in Fig. 3b, where am is plotted over $N_\tau^{-1} = aT$. Note, that the continuum limit corresponds to the origin of the plot as $am \to 0$ and $N_\tau \to \infty$. For the first-order region to be physical, the \mathbb{Z}_2 -boundary line must hence connect to the origin of the plot, i.e., the continuum. In this variable pair tricritical scaling of the \mathbb{Z}_2 -boundary takes the form

$$aT^{c}(am, N_{f}) = aT^{\text{tric}}(N_{f}) + A(N_{f})(am)^{2/5} + B(N_{f})(am)^{4/5} + O\left((am)^{6/5}\right),$$
(4)

for each N_f . In Fig. 3b we restricted the fit range to smaller masses, as we expect stronger scaling behaviour. For $N_f = 3$ and 4, we only have two data points making an extrapolation impossible. A clear support of tricritical scaling is given by $N_f = 6$ as it exhibits leading-order scaling across three lattice spacings. The case of $N_f = 8$ represents an exception and will be discussed in detail in Section 3.3. For each number of flavours, the intersection with the x-axis yields the tricritical point $aT^{\text{tric}}(N_f)$. This point marks the tricritical lattice spacing in the chiral limit where the chiral transition changes from first order ($aT > aT^{\text{tric}}$) to second order ($aT < aT^{\text{tric}}$). As our extrapolations terminate for all flavours $N_f \le 7$ at non-zero $aT^{\text{tric}}(N_f)$ – and *not* in the origin – we conclude that for all flavours $N_f \le 7$, the first-order region is merely a cutoff effect, and the transition in the continuum chiral limit is second order for all $N_f \le 7$.

Accordingly, the lattice theory differs significantly from continuum QCD in qualitative terms. We found that on the lattice, every number of flavours, $N_f \leq 7$, exhibits a tricritical point at some $aT^{\text{tric}}(N_f)$, with a clear trend of $aT^{\text{tric}} \rightarrow 0$ as N_f increases. In contrast, continuum QCD features





Figure 3: The \mathbb{Z}_2 -boundary $\{\beta_c^{\mathbb{Z}_2}, am_c^{\mathbb{Z}_2}, N_f, N_\tau\}$ projected onto different planes. Every point represents a phase boundary with an implicitly tuned $\beta_c^{\mathbb{Z}_2}(am, N_f, N_\tau)$. The lines correspond to fits according to Eq.(1) for the left panel and Eq.(4) for the right panel. On the right, dotted lines are LO-fits, while dashed lines are NLO-fits. The points for $N_f = 8$ at $N_\tau = 8$ and 10 do not correspond to the \mathbb{Z}_2 -boundary, but presumably mark the onset of the lattice bulk transition, see section 3.3.

only one unique tricritical point, $N_f^{\text{tric, phys}}$ at a = 0. Based on the qualitative behaviour shown in Fig. 3b, this *physical* $N_f^{\text{tric, phys}}$ corresponds to a (not necessarily integer) value, where the tricritical line terminates at the origin of the plot, that is, $aT^{\text{tric, phys}} = 0$. Our data suggest that this physical tricritical point must be located at $N_f^{\text{tric, phys}} > 7$. Whether this point signals the onset of first-order transitions or marks the end of chiral symmetry breaking, i.e., the beginning of the conformal window, is revealed by the corresponding temperature at that point.

3.2 Phase boundary in physical units

The temperature is calculated by introducing physical units through setting the scale in our lattice simulations. We stress that comparing QCD with different numbers of flavours requires caution as this is not merely a modification of standard bare parameters but rather a change of the entire theory. A fixed reference scale for different N_f is hence problematic. Furthermore, the understanding of units loses its conventional meaning in this setting, as our study with degenerate quarks and various N_f values departs significantly from the physical point. Our method of choice for measuring the lattice spacing is via the improved Sommer parameter r_1 [36, 37]. It is directly tied to the force between two static quarks and has proven to be robust against changes in quark mass and number of flavours [38, 39].

The calculated lattice spacings for our data of the \mathbb{Z}_2 -boundaries are shown in Fig. 4 in units of fm. We chose this representation similar to Fig. 3b, with am over $aT = N_{\tau}^{-1}$, as the connection $a \sim N_{\tau}^{-1}$ becomes directly evident. Once a is known, all other lattice observables can be converted to physical units. Thus, we derive Fig. 5 showing the mass in units of r_1 over the critical temperature in MeV. Again, we perform fits for each N_f according to our tricritical scaling ansatz

$$T^{c}(m, N_{f}) = T^{\text{tric}}(N_{f}) + A(N_{f})m^{2/5} + B(N_{f})m^{4/5} + O(m^{6/5}).$$
(5)

The tricritical points $T^{\text{tric}}(N_f)$, i.e., the intersections with the x-axis, tell us at which temperature chiral symmetry is restored in the chiral limit. Note that these are not the critical temperatures in



Figure 4: The lattice spacings of the \mathbb{Z}_2 -boundary in physical units.



Figure 5: The critical temperatures on the \mathbb{Z}_2 -boundary. The lines correspond to fits according to Eq.(5). The points for $N_f = 8$ at $N_\tau = 8$ and 10 do not correspond to the \mathbb{Z}_2 -boundary.

the continuum, but rather the transition temperatures at the tricritical points which, demonstrated in the previous section, are at finite lattice spacings aT^{tric} . Nevertheless, Fig. 5 reveals a decreasing trend in the tricritical temperature, with $T^{\text{tric}}(N_f) \rightarrow 0$ as N_f increases. In combination with the finding of the previous section, namely $aT^{\text{tric}}(N_f) \rightarrow 0$, our data is consistent with the existence of a unique (not necessarily integer) tricritical $N_f^{\text{tric, phys}}$ in the continuum with a temperature of $T(N_f^{\text{tric, phys}}) = 0$. The thus resulting picture is visualized in Fig. 6 and discussed in the conclusion.

3.3 Bulk Transition for $N_f = 8$

The analysis based on tricritical scaling for numbers of flavours $N_f \leq 7$ cannot be applied for $N_f = 8$. The reason is the occurrence of the lattice bulk transition at $N_{\tau} = 8$ and 10. This transition is a pure lattice artifact and does not correspond to a physical phase transition in the continuum. It is associated with the discretization of spacetime, not the physical continuum system, and becomes more pronounced at strong coupling (large lattice spacing). See [40-43] for details and references. The bulk transition differs from a thermal phase transition in that it is independent of the temperature, or N_{τ} . This is observed in Figures 3a and 3b, where increasing N_{τ} from 8 to 10 does not result in a change in the critical mass for $N_f = 8$. Furthermore, the critical β -values for N_{τ} = 8 and 10 are also identical (not shown). This is eventually the reason for the similar lattice spacings in Fig. 4, even though simulations were performed at different values of N_{τ} . It suggests that the critical masses at $N_{\tau} = 8$ and 10 do not correspond to a \mathbb{Z}_2 -boundary, but to the onset of the bulk transition. Determining the critical mass-value $m_c^{\mathbb{Z}_2}$ of the thermal transition is no longer within reach, as for $N_{\tau} \geq 8$, it falls below the onset of the bulk transition. For masses below the onset, we are in a bulk regime where the thermal restoration of chiral symmetry ceases to exist. Concluding, for $N_f = 8$, the thermal \mathbb{Z}_2 -line does not terminate in the chiral limit at a tricritical point, but instead ends at a non-zero mass $am^{bulk} > 0$ which is the onset of the bulk phase. There is hence no basis for tricritical scaling. Nevertheless, based on the fact that it is well established that the bulk regime is a lattice artifact and not physical, we conclude that for $N_f = 8$, the observed first-order region is again not connected to the continuum.



Figure 6: Lattice phase diagram in the chiral limit. Tricritical points $\{N_f^{\text{tric}}, T^{\text{tric}}, a^{\text{tric}}\}$ in red separate the first order from the second-order region. Only the latter is connected to the continuum a = 0.

4. Conclusion

For unimproved staggered fermions, a first-order transition exists in the chiral limit for all N_f on coarse lattices. However, this is merely a cutoff effect and terminates at a finite tricritical lattice spacing, $N_{\tau}^{\text{tric}^{-1}} = aT^{\text{tric}}(N_f)$, for all $N_f \leq 7$. It was observed that $aT^{\text{tric}} \to 0$ as N_f increases. The temperatures at these tricritical points were determined through scale setting, revealing that $T^{\text{tric}}(N_f) \rightarrow 0$ with increasing N_f . The resulting picture is presented in Fig. 6. The $T - N_f$ phase diagram in the chiral limit is extended by a third dimension being the lattice spacing. The indicated surface separates a chirally broken regime (below) from a chirally symmetric regime (above). For each lattice spacing a there is a corresponding tricritical point $N_f^{\text{tric}}(a)$. The tricritical points lie on a tricritical line indicated in red. This line marks the separation between the first-order region for large lattice spacing and a second-order region for small lattice spacing. Following the tricritical line to a = 0, it approaches the physical tricritical point $N_f^{\text{tric, phys}}$. Our data is consistent with a physical tricritical point at T = 0. In this case $N_f^{\text{tric, phys}}$ coincides with the onset of the conformal window N_f^* and marks the end of chiral symmetry breaking. Accordingly, a first-order transition in the chiral limit can be excluded for all numbers of flavours. We have not yet been able to pinpoint $N_f^{\text{tric, phys}}$. However, we have first indications for a non-integer value between 7 < $N_f^{\text{tric, phys}}$ < 8. This physical $N_f^{\text{tric, phys}}$ is then characterized by a \mathbb{Z}_2 -boundary line terminating, on the one hand, in the origin of Fig. 3b, i.e., $aT^{\text{tric}} = 0$ and, on the other hand, also in the origin of Fig. 5, i.e., $T^{\text{tric}} = 0$. For $N_f = 8$, we observe a lattice bulk transition and the absence of a tricritical point. As the bulk transition is known to be a discretization artefact, the statement remains valid that the first-order region observed on the lattice is not connected to the continuum for any N_f . This renders the transition in the chiral limit second order for all numbers of flavours unless a, so far unknown, first-order region emerges at very small lattice spacings.

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