Finite temperature QCD phase transition and its scaling window from Wilson twisted mass fermions

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Abstract. We study the properties of finite temperature QCD using lattice simulations with $N_f = 2 + 1 + 1$ Wilson twisted mass fermions for pion masses from physical up to heavy quark regime. In particular, we investigate the scaling properties of the chiral phase transition close to the chiral limit. We found compatibility with $O(4)$ universality class for pion masses up to physical and in the temperature range [120 : 300] MeV. We also discuss other alternatives, including mean field behaviour or $Z_2$ scaling. We provide an estimation of the critical temperature in the chiral limit, $T_0 = 134^{+6}_{-4}$ MeV, which is stable against various scaling scenarios.

1 Introduction

The phase diagram of Quantum Chromodynamics (QCD) has been actively investigated for many years. Nevertheless, it still contains a lot of interesting open problems. One particular question is the interplay between confinement and chiral symmetry breaking. It has been suggested that in QCD they may be related, and this belief receives some support from the observed correlation among some chiral and gauge observables. However, as it is well known, chiral symmetry is well defined only for massless quarks, and confinement can be described as a phase transition with an associated order parameter only in pure gauge systems, or, equivalently, in the infinite quark mass limit, where quarks decouple. In the intermediate region, which comprises the physical point, both phenomena are crossovers. It is then conceivable that the two phenomena are not related, and indeed there are suggestions of a possible large splitting between deconfinement and chiral symmetry restoration phase transitions, including specific quarkyonic phase [1] at high density or a possible onset of deconfinement in QCD at temperatures higher than chiral phase transition [2, 3].

In the present study we investigate chiral properties of QCD. In particular we look at the onset of the scaling window, related to the behaviour of QCD in the chiral limit $m \to 0$. Our study involves ensembles generated with Wilson twisted mass fermions for several masses,
for physical to moderately high. We plan in the future to investigate the interrelation of chiral symmetry and confinement properties, further exploiting results in our set of pion masses.

The properties of QCD in the chiral limit attract a lot of attention. They are tightly related to the fate of chiral and axial symmetry and their breaking/restoration. If the $U_A(1)$ axial symmetry remains broken after the chiral phase transition, the thermal QCD phase transition is in the three dimensional $O(4)$-universality class. If it is effectively restored at the chiral phase transition, then in the chiral limit the transition is in another universality class [4] or is the first order. In the latter case, the transition remains of first order for small nonzero quark mass, ending in a second order endpoint in the $Z_2$ universality class, for details see review of lattice results [5, 6].

Table 1. Pion masses and lattice spacings of the ensembles used in this study.

<table>
<thead>
<tr>
<th></th>
<th>M140</th>
<th>D210</th>
<th>D370</th>
<th>B270</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_\pi$ [MeV]</td>
<td>139.3(7)</td>
<td>225(5)</td>
<td>383(11)</td>
<td>376(14)</td>
</tr>
<tr>
<td>$a$ [fm]</td>
<td>0.0801(4)</td>
<td>0.0619(18)</td>
<td>0.0619(18)</td>
<td>0.0815(30)</td>
</tr>
</tbody>
</table>

Figure 1. The universal scaling behaviour for the chiral condensate and the new order parameter $\langle \bar{\psi}\psi\rangle_3$ according to $O(4)$ universality class and mean field scaling. We also present rescaled dependence of $\langle \bar{\psi}\psi\rangle_3$, going via point $(0, 1)$. Figure from [7].

We study the properties of QCD thermal phase transition for several pion masses starting from physical up to a heavy quark regime, $m_\pi \approx 400$ MeV. Particular attention is drawn to the possible scaling behaviour close to the chiral limit. We discuss possible scenarios, including $O(4)$ scaling, $Z_2$ scaling and a possible crossover to a mean field behaviour. We also provide an estimation of critical temperature in the chiral limit, which is robust under various scenarios. In [8] it was argued that critical temperature in the chiral limit is an upper bound for the temperature of the critical end point at non-zero density[8].

First results of our study were reported in [9]. A more detailed discussion can be found in [7].
2 Lattice details and studied observables

We performed simulations with \( N_f = 2 + 1 + 1 \) Wilson twisted mass fermions at maximal twist. Simulations have been carried out in a fixed scale approach. A short summary of used ensembles is presented in Tab. 1.

To study the chiral phase transition we measured the chiral condensate \( \langle \bar{\psi} \psi \rangle \) and the chiral susceptibility \( \chi = \frac{\partial \langle \bar{\psi} \psi \rangle}{\partial m} \). In order to assess possible scaling window we introduce a new order parameter[7], combining the chiral condensate and the chiral susceptibility:

\[
\langle \bar{\psi} \psi \rangle_3 = \langle \bar{\psi} \psi \rangle - m \chi,
\]

where \( m \) is the light quark mass [10]. Note that any term linear in mass in the chiral condensate cancels out in this combination. In particular, the leading order divergence \( \sim m/a^2 \), as well as any regular linear terms are absent in \( \langle \bar{\psi} \psi \rangle_3 \). Taylor expansion of \( \langle \bar{\psi} \psi \rangle_3 \) in mass in the chirally symmetric phase starts from cubic terms \( \sim m^3 \).

![Figure 2](image_url). The dependence of the pseudocritical temperature on the pion mass extracted from chiral condensate (red circles), chiral susceptibility (green rombi) and new order parameter (blue squares) together with fits by \( O(4) \) universality class. The results by Budapest-Wuppertal collaboration [11], HotQCD collaboration [12], FASTSUM collaboration [13, 14] are also presented. Green cross indicates the estimation of the critical temperature \( T_\theta = 134_{-5}^{+6} \) MeV in the chiral limit. Figure from [7].

From the universal Equation of State (EoS) for the chiral condensate

\[
\frac{\langle \bar{\psi} \psi \rangle}{m^{1/\delta}} = f(x = t/m^{1/\beta \delta}),
\]

one can easily obtain the EoS for the new order parameter

\[
\frac{\langle \bar{\psi} \psi \rangle_3}{m^{1/\delta}} = f(x)(1 - 1/\delta) + \frac{x}{\beta \delta} f'(x).
\]

Here \( \delta \) and \( \beta \) are the critical exponents, \( f(x) \) is the universal scaling function. In Fig. 1 we present the dependence of the chiral condensate and \( \langle \bar{\psi} \psi \rangle_3 \) on the scaling parameter \( x \).
Table 2. Critical temperature in the chiral limit $T_0$ extracted from three studied observables.

<table>
<thead>
<tr>
<th>Observable</th>
<th>Chiral condensate</th>
<th>Chiral susceptibility</th>
<th>$\langle \psi \psi \rangle_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_0$ [MeV]</td>
<td>138(2)</td>
<td>132(4)</td>
<td>132(3)</td>
</tr>
</tbody>
</table>

according to $O(4)$ universality class and mean field scaling. The pseudo-critical temperature extracted from the inflection point of the new order parameter corresponds to $x = 0.55(1)$, which is lower than the pseudocritical temperature determined by the inflection point of the chiral condensate, $x = 0.74(4)$. It implies that pseudo critical temperature determined from the new order parameter is closer to the critical temperature in the chiral limit. We also note that $\langle \phi \phi \rangle_3$ falls off much faster as compared to the chiral condensate in the high-temperature region: $\langle \phi \phi \rangle_3 \sim t^{-\gamma} 2^{\delta}$ and $\langle \phi \psi \rangle \sim t^{-\gamma}$.

3 Critical temperature in the chiral limit

3.1 Scaling of pseudocritical temperatures

We extract the pseudo-critical temperature from the inflection point of the chiral condensate and new order parameter $\langle \phi \phi \rangle_3$ and from the peak of susceptibility. In Fig. 2 we present the determined pseudo-critical temperatures as functions of pion mass. Apart from our results we also show the results of other groups: Budapest-Wuppertal collaboration [11], HotQCD collaboration [12], FASTSUM collaboration [13, 14]. Lines in Fig. 2 correspond to the chiral extrapolation $m \to 0$ of our data $T_c = T_0 + Am^2_\pi$ with exponents $\beta$ and $\delta$ predicted by the $O(4)$ universality class. The critical temperatures $T_0$ in the chiral limit obtained from the extrapolation are presented in Tab. 2. We note that critical temperatures, extracted from the chiral susceptibility and from the new observable $\langle \phi \phi \rangle_3$, extrapolate to the same values.
of $T_0$, while the critical temperature obtained by extrapolation of the data for the chiral condensate is slightly higher. It might indicate possible larger violations of scaling in the chiral condensate. As a final conservative estimation we take an average over all three extrapolated values:

$$T_0 = 134^{+6}_{-4} \text{ MeV.} \quad (4)$$

### 3.2 Behaviour of $\langle \bar{\psi} \psi \rangle_3$

Alternative method for the estimation of the critical temperature in the chiral limit is based on the universal behaviour of $\langle \bar{\psi} \psi \rangle_3$. According to Eq. (3), for the critical temperature at the chiral limit $t = 0$: $\langle \bar{\psi} \psi \rangle_3/m^{1/6} \sim \langle \bar{\psi} \psi \rangle_3/m^{2/6} = \text{const}$ does not depend on the pion mass. In Fig. 3 we present the rescaled data for $\langle \bar{\psi} \psi \rangle_3/m^{1/6}$ for three studied values of the pion mass. We note that all three curves go through one point, although for the largest pion mass it might be a mere coincidence. From the crossing point of the curves for two light pion masses, we obtain another estimation of the critical temperature in the chiral limit $T_0 = 138(2) \text{ MeV}$. Note that this number is in agreement with the estimation of $T_0$ obtained from the extrapolation of critical temperatures, Eq. (4).

### 4 Scaling behaviour

#### 4.1 Fitting with the $O(4)$ EoS

It would be interesting to see, whether the behaviour of the new order parameter $\langle \bar{\psi} \psi \rangle_3$ can be described by universal scaling functions. In Fig. 4 we present $\langle \bar{\psi} \psi \rangle_3$ together with the fits given by the Equation of State. Following standard reasoning, one may expect that any critical behaviour would eventually cross-over to mean field. We consider two possible scenarios: $O(4)$ universality class and mean field scaling. We note that the fits describe our data. One of the parameters of the fitting function is the critical temperature in the chiral limit $T_0$, thus within this procedure one can determine the $T_0$ using the data only for one
particular pion mass. The values of the $T_0$ determined from the fits to $O(4)$ universality class are: $T_0 = 142(2), 159(3), 174(2) \text{ MeV}$ for the pion masses $m_\pi = 139, 225$ and 386 MeV, correspondingly. Only values for the lowest pion mass are compatible with values of $T_0$ obtained from other two procedures, possibly indicating large violations to the universal scaling behaviour for pion masses $m_\pi > m_\pi^{\text{phys}}$ larger then physical. At the same time, the fits to the mean field behaviour work also pretty decently, only for the lowest pion mass there is some tension between fits and numerical results. We conclude that our data are compatible with $O(4)$ scaling for pion masses up to physical $m_\pi \leq m_\pi^{\text{phys}}$, where for large mass the agreement with $O(4)$ is likely accidental and the data are simply following a mean field behaviour.

4.2 $Z_2$ scaling

One of the alternative possible scenarios include a first order transition terminating in a critical endpoint at a critical pion mass $m_{cr}$ with $Z_2$ scaling. In Fig. 5 we present the pseudo-critical temperature versus pion mass extracted from all three observables together with the fits motivated by $Z_2$ behaviour. In the fits we constrain $m_{cr}$ to two values 50 and 100 MeV. Closeness of the critical exponent for $Z_2$ and $O(4)$ universality classes leads to very similar, almost indistinguishable behaviour of these two fits. For this reason, we cannot exclude the possibility of $Z_2$ scaling with some critical pion mass up to a physical $m_{cr} \leq m_\pi$. On the positive side, the extrapolated predictions for the (pseudo)-critical temperatures for $O(4)$ and $Z_2$ scenarios are very close to each other.

4.3 High temperature behaviour

![Figure 6](https://example.com/figure6.png)

**Figure 6.** New order parameter $\langle \bar{\psi} \psi \rangle_3$ divided by $m_\pi^6$. Lines correspond to the $O(4)$ high-temperature fit in the range $[160 : 300] \text{ MeV}$. At temperatures higher than 300 MeV points fall onto one curve, indicating behaviour described by leading order Griffith analyticity.
At large temperatures $\langle \bar{\psi} \psi \rangle_3$ falls off quite fast: $\langle \bar{\psi} \psi \rangle_3 \sim t^{-\gamma-2\delta}$. In Fig. 6 we present the fits of the new observables to this function in the range $[160 : 300]$ MeV, which describe data quite well. In the fit we have fixed critical temperature in the chiral limit $T_0 = 138$ MeV. At the temperature $T \sim 300$ MeV this behaviour changes, giving way to a leading order Griffith analyticity $\langle \bar{\psi} \psi \rangle_3 \sim m^3 \sim m^6$, thus rescaled $\langle \bar{\psi} \psi \rangle_3/m^6$ lie on one curve for temperatures $T > 300$ MeV. Remarkably, in the previous paper [15] temperature $T \sim 300$ MeV was found to be an onset of the dilute instanton gas behaviour. The existence of possible thresholds in quark-gluon plasma has been actively discussed in several works [3, 16, 17]. In particular, in [3] it was proposed that $T \sim 300$ MeV can be a pseudo-critical temperature for magnetic monopole condensation, which may be associated with the confinement-deconfinement phase transition. We plan to study the possible connection of the observed upper boundary of the scaling window with confinement properties in the future.

In Fig. 7 we sketch the $O(4)$ scaling window consistent with our results: it extends for temperatures from 120 MeV to 300 MeV and pion masses up to physical $m_\pi \approx m_\pi^{\text{phys}}$.

![Figure 7. Sketch of the O(4) scaling window consistent with the results of our simulations. Blue points indicate the (pseudo)critical temperatures extracted determined from the new observable for the studied pion masses and in the chiral limit. Figure from [7].](https://doi.org/10.1051/epjconf/202225805012)

5 Conclusions

The properties of QCD and its thermal phase transition have been the subject of various studies. In this Proceeding we present the results of our lattice study of finite temperature...
QCD with $N_f = 2 + 1 + 1$ Wilson twisted mass fermions for pion masses from physical up to heavy quark regime. We propose a novel order parameter (1), which is free from linear terms in mass and turns out to be quite useful for study of the scaling behaviour. We measured the pseudo-critical temperatures and made an extrapolation to the chiral limit, $T_0 = 134^{+6}_{-4}$ MeV. An alternative method, based on the scaling properties of the new observable, picks up slightly larger value $T_0 = 138(2)$ MeV, although compatible within errorbars. The dependence of the new order parameter on the temperature can be described by $O(4)$ universal functions, however only for the lowest pion mass $m_\pi = 139.3(7)$ MeV the extracted value of $T_0$ is compatible with previous estimation. At the same time, our data can be described by mean field motivated fits, only for the lowest pion mass there is a tension between the fits and our data. Based on this we conclude that our data are compatible with $O(4)$ universality class for temperatures in $[120, 300]$ MeV and pion masses up to physical, although an alternative scenario, based on $Z_2$ scaling, cannot be ruled out. We sketch our estimation of the $O(4)$ scaling window in Fig. 7.

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The work is partially supported by STRONG-2020, a European Union’s Horizon 2020 research and innovation programme under grant agreement No. 824093. A.Yu.K. and A.T. acknowledge support from RFBR grant 18-02-40126. A.T. was supported by the "BASIS" foundation. Numerical simulations were carried out using computing resources of CINECA (based on the agreement between INFN and CINECA, on the ISCRA project IsB20), the supercomputer of Joint Institute for Nuclear Research “Govorun”, and the computing resources of the federal collective usage center Complex for Simulation and Data Processing for Megascience Facilities at NRC “Kurchatov Institute”, http://ckp.nrcki.ru/.

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References