Finite temperature QCD with $N_f = 2 + 1 + 1$ Wilson twisted mass fermions at physical pion, strange and charm masses

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Abstract We discuss recent progress in studying Quantum Chromodynamics at finite temperature using $N_f = 2 + 1 + 1$ Wilson twisted mass fermions. Particular interest is in QCD symmetries and their breaking and restoration. First, we discuss the behaviour of the $\eta'$ meson at finite temperature, which is tightly connected to the axial and chiral symmetries. The results suggest a small decrease of the $\eta'$ mass in the pseudo-critical region coming close to the non-anomalous contribution and subsequent growth at large temperatures. Second, we present the first results of lattice simulations of Quantum Chromodynamics with $N_f = 2 + 1 + 1$ twisted mass Wilson fermions at physical pion, strange and charm masses. We estimate the chiral pseudo-critical temperatures for different observables. Our preliminary results are consistent with a second order transition in the chiral limit, however other scenarios are not excluded.

1 Introduction

Quantum Chromodynamics under extreme conditions has been the subject of numerous theoretical and experimental studies [1]. In the experiments on heavy ion collisions at Relativistic Heavy Ion Collider, Brookhaven and Large Hadron Collider, CERN a droplet of strongly coupled matter at large temperatures is believed to be produced, thus providing a great opportunity to study thermal QCD. One of the most famous experimental discoveries was the observation of the Quark-Gluon Plasma — a new state of matter, characterized by unbound deconfined quarks and gluons. From the theoretical side, the existing information on finite temperature QCD is based on first-principle lattice supercomputer simulations, see e.g. Ref. [2] for a recent review.

Properties of strongly interacting matter at nonzero temperature are tightly related to the symmetries and symmetry breaking pattern of QCD [3]. The chiral symmetry $SU_L(2) \times SU_R(2)$, being broken in the vacuum state of QCD, becomes effectively restored at temperature $T_c \approx 160$ MeV [4–6]. Approximately at the same temperature the transition to the deconfined phase of Quark-Gluon Plasma occurs with both transitions being analytical crossovers, rather than the phase transitions [7].

The behaviour of $U_A(1)$ axial symmetry at finite temperature is a more subtle issue. The proposed mechanism of instanton suppression might lead to the effective restoration of the axial symmetry close to the chiral (pseudo-)critical temperature [8]. Numerical lattice studies of various observables with different fermion discretisations give rather controversial results — some propose joint effective restoration of axial and chiral symmetry, while others favour axial symmetry restoration at much higher temperatures (see [3] and references therein). From a phenomenological point of view, the restoration of axial symmetry should be reflected in the particle spectrum as a degeneracy of axial partners, see [9] and references therein.

The behaviour of $U_A(1)$ symmetry also has a clear link to the universality class of the finite temperature QCD phase transition [10,11]. If it remains broken after the chiral phase transition, the transition in the chiral limit should be in the $O(4)$-universality class. Effective restoration of $U_A(1)$ implies enlarged symmetry breaking pattern and, consequently, another behaviour of the chiral transition: it should be either first-order or in the other universality class $U(2) \otimes U(2)/U(2)$. The scaling of chiral observables with

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the quark mass could in principle distinguish possible scenarios, thus calling for simulations at low pion mass, even lower than physical [12].

Apart from axial and chiral symmetry restoration, the existence of other thresholds in Quark-Gluon Plasma was proposed [13,14] suggesting possible emergence of more elaborate symmetries. So far, the thermal QCD and its symmetries and symmetry breaking patterns are not yet fully understood and further first-principle results are required.

In this note we present lattice results in the Wilson twisted mass discretization at maximal twist, with two families of quarks. The strange and charm masses are set at their physical values, while the light (degenerate) quarks take different values, including the physical one. The gauge field configurations were generated using the public ETMC code. Our setup for pion masses ranging from 210 MeV till 470 MeV is taken from Ref. [15], while for the physical pion mass we use the recent tuning of Refs. [16,17].

2 $\eta'$ and QCD symmetries

The behaviour of the axial and chiral symmetries in Quantum Chromodynamics is tightly connected with the meson spectrum. Spontaneous breaking of chiral symmetry leads to an octet of Goldstone bosons: $\pi$‘s, $K$‘s and $\eta$. Nonzero quark masses $m_q$, breaking chiral symmetry explicitly, lead to small nonzero masses of these pseudo-Goldstone bosons $M^2_{\pi, K, \eta} \sim m_q \Lambda_{QCD}$. If $U_A(1)$ axial symmetry would be also spontaneously broken, its would-be Goldstone boson $\eta'$ mass should follow the same pattern. However, the experimental result for $m_{\eta'} \sim 1$ GeV is much higher than the masses of the octet of pseudoscalar mesons. The solution to this well known puzzle comes from the fact that the axial symmetry is anomalously broken and $\eta'$ mass gets an additional contribution coming from axial anomaly [19]. This contribution can be quantitatively taken into account within large-$N$ limit [20]. There are studies of the $\eta/\eta'$-complex beyond large-$N$ approximation, both phenomenological [21] and on the lattice [22–26]. In general, the behaviour of the $\eta'$ in QCD at zero temperature is well understood (see, e.g., the detailed discussion in [9]). The properties of $\eta'$ at finite temperature are less clear and require first-principle investigation.

To determine the $\eta'$-mass at nonzero temperature we measured the correlator of the topological charge density $G^q(t) = \int d^3x \langle q(\bar{x}, t)q(0, 0) \rangle$, which is coupled to $\eta'$ due to the axial anomaly. Topological charge density was measured with the help of Gradient Flow [27]. By fitting the data at large Euclidean times with a simple behaviour $G(t) \sim \cosh [m(t - N_t/2)]$, where $N_t$ is the temporal lattice extent, we extracted the parameter $m$, which corresponds to the $\eta'$ mass. More detailed description of the simulation setup can be found in our original paper [9]. The final results for the temperature dependence of the $\eta'$-mass for two pion masses $m_\pi = 370$ MeV and $m_\pi = 210$ MeV are presented in Fig. 1.

The results suggest a small decrease in the $\eta'$ mass in the vicinity of the chiral pseudo-critical temperature followed by an increase at larger temperatures. Various phenomenological studies [28–33] provide similar trend, although some quantitative features are different. One of the possible explanation of these results would be the restoration of chiral and axial symmetries, so that the whole nonet of pseudo-Goldstone bosons becomes degenerate. To draw more definite conclusions, one needs more information from other observables, sensitive to chiral and axial symmetry. In particular, it is very important to measure the spectrum of other particles, both already mentioned pseudo-Goldstone bosons as well as other mesons, at finite temperature, and to extend the results to physical pion mass. This is the subject of an ongoing study.

3 Chiral phase transition for physical pion mass

One of the challenges of modern lattice studies of QCD is related to the fact that the required computational time grows very fast with the pion mass going down to its physical value. So far, the main results at the physical pion mass $m_\pi \sim 140$ MeV were obtained for (improved) staggered fermions [4,5], although results with other discretizations are also available [34]. One of the alternatives is to use Wilson-type fermions, in particular, twisted-mass implementation of Wilson fermions [35]. Development of multi-grid algorithm [36] made it possible to perform simulations with twisted mass fermions at physical pion mass.

Our setup is based on recent tuning of the parameters by ETM collaboration at $T = 0$ for physical pion mass [16,17].
Following Refs. [16, 17], simulations were performed with $N_f = 2 + 1 + 1$ Wilson twisted mass fermions at the isospin symmetric point. With respect to our previous study, a clover term was included, and the fermionic action for two light quarks $S^l$ and for $1 + 1$ heavy doublet $S^h$ has the following form:

$$
S^l = \sum_{x,y} \bar{\chi}_l(x) \left[ 1 - i \frac{1}{2} c_{SW} \sigma^{\mu \nu} F_{\mu \nu} \right] \delta_{x,y} - \kappa D_W[U](x,y) + 2i \mu_1 \tau^1 \gamma^5 \delta_{x,y} \chi_l(y),
$$

$$
S^h = \sum_{x,y} \bar{\chi}_h(x) \left[ 1 - i \frac{1}{2} c_{SW} \sigma^{\mu \nu} F_{\mu \nu} \right] \delta_{x,y} - \kappa D_W[U](x,y) + 2i \mu_1 \tau^1 \gamma^5 \delta_{x,y} + 2k \mu_2 \tau^3 \delta_{x,y} \chi_h(y),
$$

where $a$ is the lattice spacing, $D_W[U]$ is the usual Wilson operator, $c_{SW} \sigma^{\mu \nu} F_{\mu \nu}$ is the standard clover term [37].

For the gauge fields the Iwasaki improved action was used ($c_0 = 3.648, c_1 = -0.331$):

$$
S^g = \beta \sum_p \left( c_0 \sum_p \left[ 1 - \frac{1}{3} \Re \Tr U_p \right] + c_1 \sum_R \left[ 1 - \frac{1}{3} \Re \Tr U_R \right] \right).
$$

Here $\sum_p$ and $\sum_R$ denote the sum over all $1 \times 1$ plaquettes and over all $1 \times 2$ rectangles, correspondingly. Parameters of the action were tuned by zero temperature simulations of ETM collaboration [16] to reproduce physical pion mass $m_\pi = 139.3(7)$ MeV [38]. We summarize the parameters used in our simulations in Table 1.

Simulations are performed in a fixed-scale approach, where temperature $T = \frac{1}{N_t a}$ is varied by varying the temporal extent of the lattice $N_t$, and all the parameters of the action (1)–(2) are kept constant. Used bare parameters correspond to the lattice spacing $a = 0.0801(4)$ fm [38]. Spatial lattice size was fixed $N_s = 64$, or $N_s a = 5.126(26)$ fm. During generation each 4th trajectory was saved. Summary of all used statistics for various values of $N_t$ is presented in Table 2. Simulations are still in progress, and complete results will be reported elsewhere.

In our first study with $N_f = 2 + 1 + 1$ twisted mass fermions at physical pion mass we measured simple chiral observables: the light quark chiral condensate $\langle \bar{\psi} \psi \rangle$ and the disconnected chiral susceptibility $\chi_{\bar{\psi} \psi}^{\text{disc}} = \frac{V}{T} \left( \langle \bar{\psi} \psi \rangle^2 \rangle - \langle \bar{\psi} \psi \rangle \right)$. In Table 2 we also present the data for these observables. The statistical errors were measured by $\Gamma$-method [42]. The typical autocorrelation time for studied observables was $\sim 1$ configuration far from pseudocritical temperatures and $\sim 3$ configurations for temperatures $T$ near $T_c$ and was taken into account in error analysis. Using their temperature dependence we estimated the pseudocritical temperature of the chiral phase transition, as the inflection point of the chiral condensate $\langle \bar{\psi} \psi \rangle$ versus $T$ and the peak in the susceptibility $\chi_{\bar{\psi} \psi}^{\text{disc}}$. To extract the inflection point $T_{\Delta}$, the chiral condensate in the transition region was fitted by several functions $\langle \bar{\psi} \psi \rangle = A + B \tan \frac{T - T_{\Delta}}{(T_{\Delta})}$, $\langle \bar{\psi} \psi \rangle = A + B (T - T_{\Delta}) / \sqrt{T_{\Delta}^2 + (T - T_{\Delta})^2}$ and $\langle \bar{\psi} \psi \rangle = a_{\Delta} + b_{\Delta} T + c_{\Delta} T^2 + d_{\Delta} T^3$. The difference of $T_{\Delta}$ extracted from various fits, and by varying fitting interval, allowed us to estimate the systematic uncertainty of our results. In the same way by using various functions $\chi_{\bar{\psi} \psi}^{\text{disc}} = A_0 + B_0 (T - T_{\Delta})^2$.

### Table 1 Parameters of the action (1) and (2)

| $N_t$ | $\beta$ | $c_{SW}$ | $\kappa$ | $\mu_1$ | $\mu_\sigma$ | $\mu_\delta$ |
|-------|---------|----------|----------|---------|-------------|-------------|
| 64    | 1.778   | 1.69     | 0.1394265| 0.00072 | 0.1246864   | 0.1315052   |

Simulations are performed in a fixed-scale approach, where temperature $T = \frac{1}{N_t a}$ is varied by varying the temporal extent of the lattice $N_t$, and all the parameters of the action (1)–(2) are kept constant. Used bare parameters correspond to the lattice spacing $a = 0.0801(4)$ fm [38]. Spatial lattice size was fixed $N_s = 64$, or $N_s a = 5.126(26)$ fm. During generation each 4th trajectory was saved. Summary of all used statistics for various values of $N_t$ is presented in Table 2. Simulations are still in progress, and complete results will be reported elsewhere.

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### Table 2 Statistics and raw data for the chiral condensate $\langle \bar{\psi} \psi \rangle$ and the disconnected susceptibility $\chi_{\bar{\psi} \psi}^{\text{disc}}$

| $N_t$ | $T$ [MeV] | $\# \text{ conf}$ | $\langle \bar{\psi} \psi \rangle$ | $\chi_{\bar{\psi} \psi}^{\text{disc}}$ |
|-------|-----------|-------------------|-----------------|-----------------|
| 20    | 123(1)    | 244               | 0.00833(5)      | 0.97(22)        |
| 18    | 137(1)    | 155               | 0.00777(11)     | 1.55(32)        |
| 16    | 154(1)    | 364               | 0.00664(9)      | 1.51(14)        |
| 14    | 176(1)    | 129               | 0.00413(7)      | 0.53(11)        |
| 12    | 205(1)    | 263               | 0.003437(15)    | 0.093(21)       |
| 10    | 246(1)    | 205               | 0.003167(4)     | 0.09(5)         |
| 8     | 308(2)    | 360               | 0.0030385(4)    | 5.1(8)\times10^{-5} |
| 6     | 411(2)    | 195               | 0.00291805(17)  | 4.4(5)\times10^{-6} |
| 4     | 616(3)    | 472               | 0.00268258(5)   | 9.6(8)\times10^{-7} |
temperatures \( T_c \) (red squares) versus the pion mass. The data for higher than physical pion masses are taken from [39]. Along with our results we present the staggered continuum extrapolated results of Wuppertal–Budapest collaboration both for \( T_\Delta \) and \( T_X \) (cyan and orange triangles) [40], recent continuum extrapolated combined for various observables results of HotQCD collaboration both at physical pion mass [5] and in the chiral limit [12] (purple rhombi) and preliminary results of the FASTSUM collaboration for \( T_\Delta \) (blue stars) [41].

In the same plot we show the (continuum extrapolated) \( T_\chi \) (green circles) and peak of the susceptibility \( \Delta \chi \) (cyan and orange triangles) [40], recent results for the physical pion mass obtained with staggered fermions [39]. In the same plot we show the (continuum extrapolated) \( T_\chi \) (green circles) and peak of the susceptibility \( \Delta \chi \) (cyan and orange triangles) [40].

Recent progress in algorithms and supercomputers leads to significant advance in first-principle lattice simulations. In this work we have presented the first results for a physical pion mass with twisted mass Wilson fermions. Our first results for the pseudo-critical temperature with \( N_f = 2 + 1 + 1 \) twisted mass fermions at physical pion mass are consistent with an \( O(4) \) universality class as found with staggered fermions [6].

However, the properties of Quantum Chromodynamics at nonzero temperature still are not yet fully understood. The properties of the chiral transition, its behaviour and universality class in the chiral limit, and the role of the axial symmetry near the chiral phase transition remain an open issue and require further attention. Although our results for the \( \eta' \) mass are in favour of disappearance of axial anomaly and restoration of the axial symmetry in the vicinity of the chiral phase transition, a more thorough study of various observables is required to draw more definite conclusions. In particular, in the future, alongside with a more complete analysis of the scaling properties of the order parameters, a detailed study of meson spectrum for physical pion mass is planned [43].

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### Data Availability Statement

This manuscript has no associated data or the data will not be deposited. [Authors’ comment: Please note that new data of this manuscript is presented in the Table 2.]

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