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Twisted mass QCD at finite temperature

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We discuss the use of Wilson fermions with twisted mass for simulations of QCD thermodynamics. As a prerequisite for a future analysis of the finite-temperature transition making use of automatic $\mathcal{O}(a)$ improvement, we investigate the phase structure in the space spanned by the hopping parameter κ, the coupling β, and the twisted mass parameter μ. We present results for $N_f = 2$ degenerate quarks on a $16^3 \times 8$ lattice, for which we investigate the possibility of an Aoki phase existing at strong coupling and vanishing μ, as well as of a thermal phase transition at moderate gauge couplings and non-vanishing μ.

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1. Introduction

Wilson fermions with a twisted mass term evaluated at "maximal twist" offer a number of advantages over untwisted fermions, such as the absence of exceptional configurations and automatic $\mathcal{O}(a)$ improvement. In order to see whether these features can also be successfully exploited for future analyses of the QCD finite temperature phase transition, we present as a prerequisite an investigation of the phase diagram spanned by the hopping parameter κ, the twisted mass parameter μ and the gauge coupling β for $N_f = 2$ quarks.

The twisted mass action for two degenerate fermions consists of the standard Wilson action, augmented by a twisted mass term $\overline{\psi} i\mu\gamma_5\tau^3\psi$. The hopping parameter κ and the twist parameter μ are related to the bare quark mass as

$$m_q = \sqrt{\frac{1}{4}\left(\frac{1}{\kappa} - \frac{1}{\kappa_c}\right)^2 + \mu^2}. \tag{1.1}$$

For maximal twist we have $\kappa = \kappa_c$, in which case the quark mass is determined by μ alone. For a recent review of the twisted mass formulation, see [1].

The expected phase structure is based on symmetry arguments and leading order chiral perturbation theory [2, 3, 4]. It has recently been discussed in [5], a qualitative sketch is shown in Figure 1. The phase diagram divides into two regions. The expected Aoki phase for small values of β (cf. [6]) is in the $\mu = 0$ plane, since $\mu \neq 0$ explicitly breaks the associated parity-flavour symmetry. For larger values of β, a conical surface is believed to mark the thermal transition between the hadronic and quark gluon regimes. This is based on the expectation [5] that, for fixed β, the lines of equal bare quark mass in the (κ, μ) plane given by equation (1.1) should correspond to lines of constant physics at that lattice spacing.

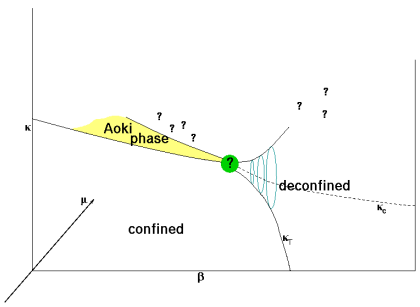

Figure 1: Speculative phase structure for twisted mass Wilson fermions. The Aoki phase is part of the $\mu = 0$ plane and the thermal transition is expected to be located on a conical surface; cf. [5].

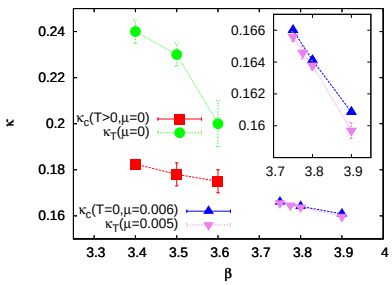

Figure 2: Summary of results. Note that the left part of the diagram shows the $\mu = 0$ plane whereas the right part (also the enlarged insert) shows the thermal transition line for $\mu = 0.005$.

Our simulations are performed on a $16^3 \times 8$ lattice using an improved HMC code as described in [7], based on the tree-level Symanzik improved gauge action. We search for signatures for the Aoki phase and its possible decoupling from the deconfinement transition in the range from $\beta = 3.40$ to 3.60. For larger β, we present results for the slice of the surface at fixed $\mu = 0.005$ obtained from simulations at $\beta \in \{3.75, 3.775, 3.8\}$, supplemented by data at $\beta = 3.9$ from a previous investigation [8]. Our findings, to be discussed in the following sections, are summarized in Figure 2.

2. Search for the Aoki Phase

In a first attempt to roughly estimate a region of parameter space for a potential Aoki phase, we performed a scan in κ at several values of β keeping $\mu = 0$ fixed. According to the Aoki phase scenario the masses of the charged as well as the neutral pions vanish along the border of the Aoki phase. Consequently, we expect the average number of conjugate-gradient iterations $\langle N_{CG}\rangle$ in the HMC process to peak there. Such a behaviour is demonstrated in the lower-left graph of Figure 3 where $-\log\langle N_{CG}\rangle$ is shown as a function of κ for different values of β. We find that the minimum of $-\log\langle N_{CG}\rangle$ shifts slightly towards lower κ as β increases. In the upper-left panel of Figure 3, this is consistently reflected in the behaviour of the average plaquette, showing a rather rapid change when approaching the region where $\langle N_{CG}\rangle$ peaks. Therefore, given the data of $\langle N_{CG}\rangle$, a possible Aoki phase should lie within the narrow interval $\kappa \in [0.16, 0.20]$.

The Polyakov loop as an indicator for a thermal phase transition remains flat throughout this interval. A significant rise can only be found for $\kappa \geq 0.21$, i. e. well beyond the possible Aoki phase region. This can be seen on the right hand side of Figure 3 where the real part of the Polyakov loop and its susceptibility are shown as functions of κ. Therefore, if an Aoki phase were found somewhere between $\kappa = 0.16$ and 0.20, this would be in contrast to the experience gained in previous investigations (with Wilson gauge action) [6] in which no clear separation of the Aoki phase from the thermal transition has been observed. As expected for the phase diagram at $\mu = 0$, the κ value at which the Polyakov loop rises significantly shifts to lower values when β is increased.

At $\beta = 3.4$ we have started a more thorough investigation of the existence of a phase of broken parity-flavour symmetry by searching for a κ-region where the order parameter $\langle\bar{\psi}i\gamma_5\tau^3\psi\rangle$ does not vanish in the limit $\lim_{h\to 0}\lim_{V\to\infty}\langle\bar{\psi}i\gamma_5\tau^3\psi\rangle$. Here the strength of the "external field" h is related to the twisted mass parameter μ by $h = 2\kappa\mu$. So far, we have only measured the order parameter as a function of κ at $\beta = 3.4$ and the three values $h = 0.01$, 0.005 and 0.0025. Our current results for the average plaquette and the order parameter are shown in Figure 4; on the left hand side both observables as functions of κ and on the right hand side only $\langle\bar{\psi}i\gamma_5\tau^3\psi\rangle$ versus h. As above, the average plaquette exposes a rapid change or discontinuity as a function of κ. This becomes slightly stronger with decreasing h. The order parameter is observed to peak around $\kappa^* \approx 0.1825$. This peak becomes smaller and narrower in width as h decreases. Looking at the right hand side of Figure 4, we get strong indications that for $h \to 0$ the order parameter tends to zero for all κ values considered. Therefore, our yet preliminary results at $\beta = 3.4$ point to an absence of the Aoki phase and a possible first order phase transition, a scenario sustained by the occurence of long-lasting metastable states at $\kappa = 0.1830$. In this context it should be mentioned that first order behaviour for Wilson fermions in the intermediate coupling regime has been observed before (cf. [9] and references therein). We interprete our data in the same way as a remnant of the $\kappa_c(T = 0)$ bulk transition. Of course, the existence of an Aoki phase at smaller β is left open. In any case, our results for the Polyakov loop show that the deconfining transition happens at considerably larger κ values.

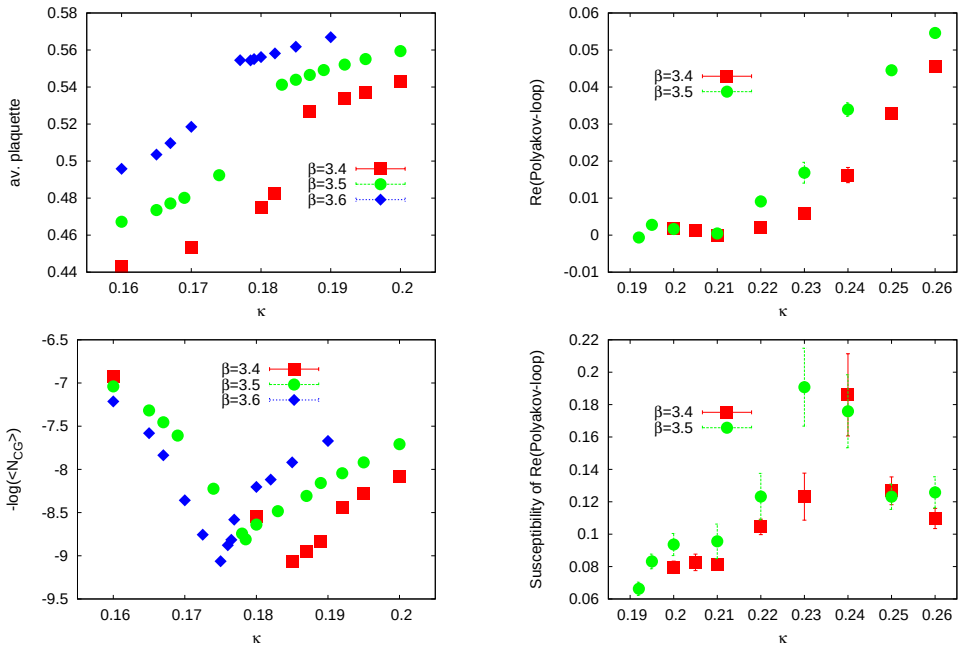

Figure 3: Scan of the phase diagram at $\mu = 0$ looking for signals of an Aoki phase. **Left:** Average plaquette (top) and minus the logarithm of the average number of CG-iterations (bottom) as functions of κ. **Right:** The real part of the Polyakov loop (top) and its susceptibility (bottom) also as functions of κ.

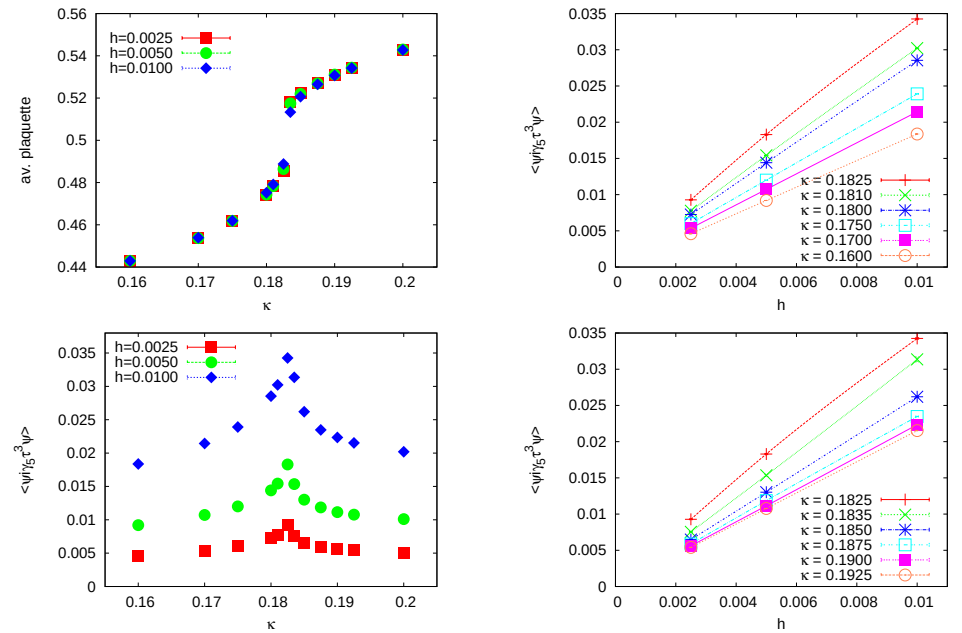

Figure 4: Search for the Aoki-phase at $\beta = 3.4$ at 3 different values of h. **Left:** Average plaquette (top) and the order parameter (bottom) versus κ. **Right:** The order parameter versus h for $\kappa \leq \kappa^*$ (top) and $\kappa \geq \kappa^*$ (bottom).

3. Thermal Transition Line

In order to locate the thermal transition line for $\mu = 0.005$ we fixed β and scanned in κ, reaching $\mathcal{O}(10000)$ statistics for each pairing. As observables we used the plaquette, the real part of the Polyakov loop and their respective susceptibilities as well as the pion norm, which is given by $\|\pi\|^2 = \sum_x \mathrm{Tr}\,\overline{\psi}(x)\gamma_5\psi(x)\overline{\psi}(0)\gamma_5\psi(0)$. The susceptibilities have been normalized as $\chi_O = N_s^3\left(\langle O^2\rangle - \langle O\rangle^2\right)$. The critical coupling κ_T for the thermal transition is then signalled by a peak in the susceptibilities.

In Figure 6 we present our data for the search for the thermal transition line at $\mu = 0.005$ for the various values of β. The critical κ_T of the transition is decreasing with growing β. This is consistent with the fact that $T_c(m)$ is an increasing function of quark mass, as found with staggered or untwisted Wilson fermions (for a recent review, see [10]). Correspondingly, the signal in the Polyakov loop becomes more pronounced with increasing β, whereas the signal in the plaquette becomes broader. The values we extracted for the thermal transition $\kappa_T(\mu,\beta)$ are collected in Figure 5; they are compared to the values for $\kappa_c(T=0,\beta)$, cf. [11, 12, 13]. As in the case of untwisted Wilson fermions [14], the distance between κ_T and κ_c grows with increasing β.

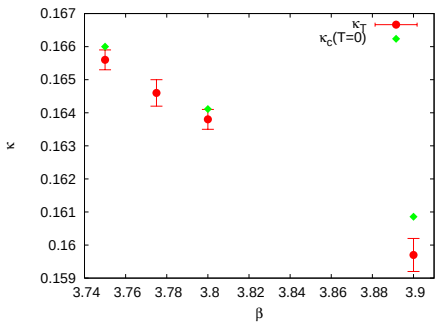

Figure 5: Results for the thermal transition line $\kappa_T(\beta,\mu=0.005)$ compared to the known points for the critical κ_c at $T=0$.

β	$\kappa_T(\beta,\mu=0.005)$	$\kappa_c(T=0,\beta)$
3.75	0.1656(3)	0.1660(1)
3.775	0.1646(4)	–
3.8	0.1638(3)	0.164111
3.9	0.1597(5)	0.160856

As stated above, due to equation (1.1), for fixed lattice spacing, viz. coupling β, there should be a line of equal physics in the (κ,μ) plane. This leads to the expectation of a conical thermal transition surface in the phase diagram as sketched in Figure 1. In order to check this expectation we have scanned for the transition both in κ for fixed μ, as well as in μ for fixed κ.

In Figure 7 we present the comparison of a scan in μ that was performed at $\kappa = \kappa_c(T=0,\beta=3.9)$ with $\mathcal{O}(4000)$ statistics with a scan in κ at $\beta = 3.9$ and $\mu = 0.005$ with up to $\mathcal{O}(10000)$ HMC sweeps. The points are mapped to an effective bare quark mass using equation (1.1). The similar behaviour provides preliminary evidence for the existence of at least part of the conical structure of the transition surface. Note that the data correspond to different μ-values. Since this varying of μ, i. e. of the twist angle $\arctan(\mu/(m-m_c))$, introduces $O(a)$ effects, the data are distorted away from the unique curve by finite lattice spacing effects.

In Figure 8 we sketch an approximate slice of the phase diagram in Figure 1 at a larger β. A line of equal critical mass, defined by (1.1), for the thermal transition is sketched. The vertical line within the ellipse is the 1^{st} order line containing $\kappa_c(\beta,T=0,\mu=0)$ as predicted by χPT for $T=0$ – cf. [3]. Our present and planned future investigations are illustrated as well.

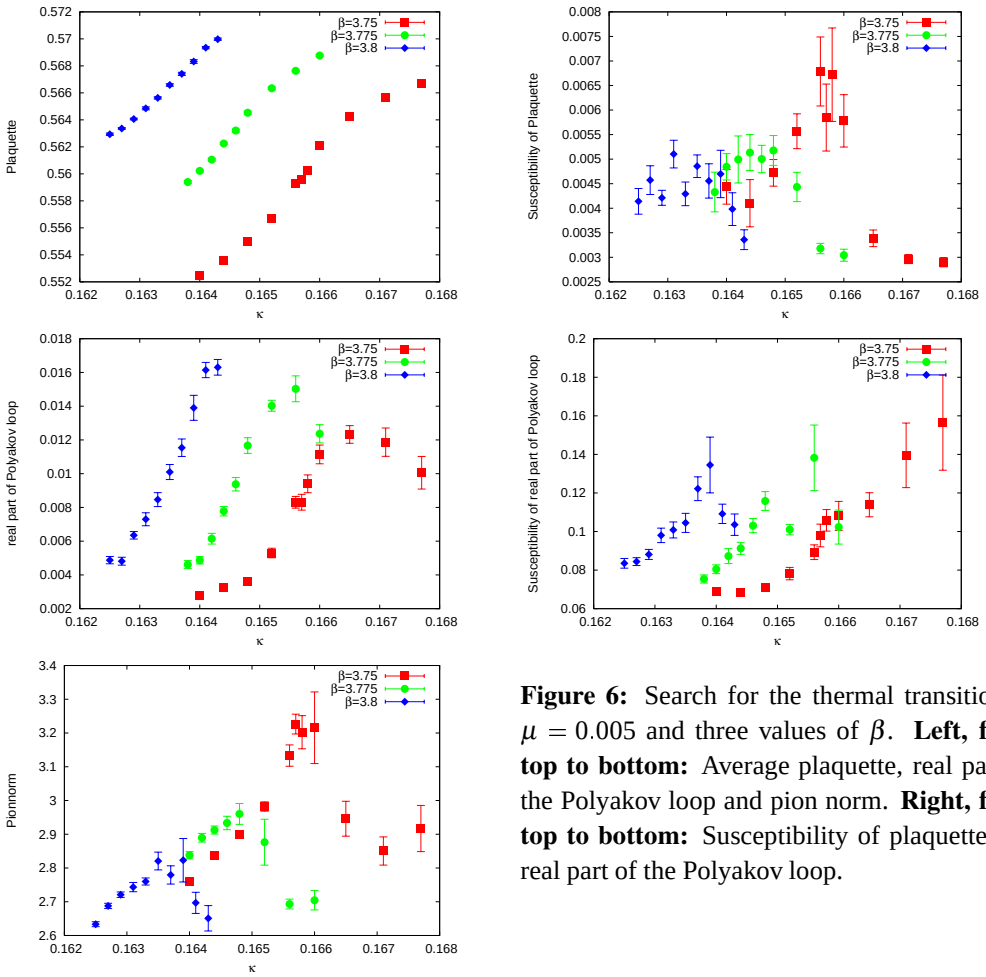

Figure 6: Search for the thermal transition at $\mu = 0.005$ and three values of β. **Left, from top to bottom:** Average plaquette, real part of the Polyakov loop and pion norm. **Right, from top to bottom:** Susceptibility of plaquette and real part of the Polyakov loop.

4. Summary and Outlook

For $\beta = 3.4$ and $\mu = 0$ we have found a very narrow range of κ-values where we observe indications for a first order phase transition similar to the bulk transition seen in the zero-temperature case. There seems to be no Aoki phase in this range of the phase diagram. The deconfinement transition occurs at considerably higher κ-values.

For larger β we have identified the thermal transition line at $\mu = 0.005$, and provided some evidence for one side of the conical phase boundary predicted in [5].

Our future work will consist of a continued investigation of the strong coupling region at β-values substantially lower than presented here as well as probing the details of the conical structure for larger β. Finally, we would like to study the thermal transition at maximal twist and to work towards physical quark masses and the continuum in this regime.

Acknowledgments

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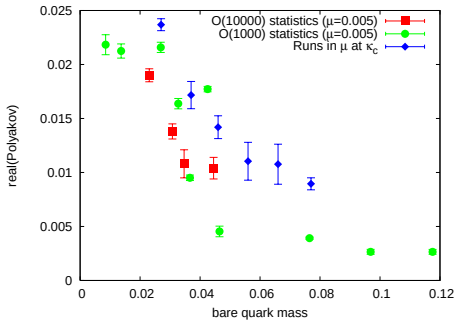

Figure 7: Comparison of runs for different (κ, μ) pairs at $\beta = 3.9$ mapped to the bare quark mass.

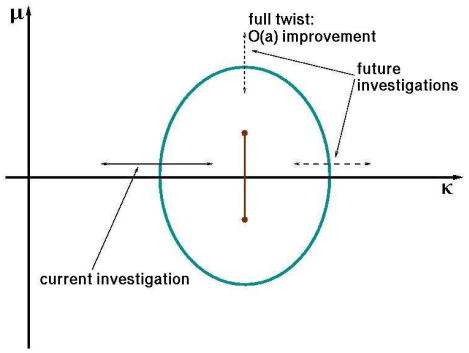

Figure 8: Current and planned investigations in the context of the expected phase structure.

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