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On the phase structure of twisted mass lattice QCD

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Abstract: The introduction of a chirally twisted mass term has been proposed as an attractive approach to $O(a)$ improvement of Quantum Chromodynamics with Wilson fermions on a lattice. For numerical simulation projects it is important to know the phase structure of the theory in the region of small quark masses. We study this question in the framework of chiral perturbation theory. Generalizing the analysis of Sharpe and Singleton we find extensions of normal and Aoki phase scenarios and a possible new phase with spontaneous breakdown of chiral symmetry to a discrete Z_2.

Keywords: Lattice Quantum Field Theory, QCD, Lattice QCD, Chiral Lagrangians.

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1. Introduction

In numerical simulations of Quantum Chromodynamics on a lattice one of the most important issues is to reduce lattice artifacts in order to improve the approach to the continuum limit. Recently the lattice formulation of QCD with Wilson fermions and a chirally twisted quark mass matrix [1, 2] has attracted much interest in this respect. Frezzotti and Rossi [3, 4] have advocated this approach as a way to remove lattice artifacts to first order in the lattice spacing a by a suitable choice of the chiral twist. Exploratory numerical studies [5] have shown favourable algorithmic features of simulations of twisted mass lattice QCD.

A prerequisite to any numerical simulation project is the knowledge of the phase structure of the model under consideration. Where are lines or points of phase transitions of first or higher order and how do physical quantities like particle masses behave near them? It is the purpose of this note to discuss the phase structure of twisted mass lattice QCD on the basis of chiral perturbation theory. Similar considerations have been made independently by Sharpe and Wu [6, 7].

We consider lattice QCD with $N_f = 2$ quark flavours and degenerate quark masses m. Let m_c be the "critical" value of m, where the quark condensate has a discontinuity, and

$$\tilde{m} = m - m_c \tag{1.1}$$

be the subtracted quark mass. The chirally twisted mass term can be introduced in the socalled "twisted basis" in the form $\bar{q}(m_c + M(\omega))q$ with

$$M(\omega) = m_q \mathrm{e}^{\,\mathrm{i}\,\omega\gamma_5\tau_3} = \tilde{m} + \mathrm{i}\,\mu\gamma_5\tau_3\,, \tag{1.2}$$

where

$$\tilde{m} = m_q \cos(\omega)\,, \qquad \mu = m_q \sin(\omega)\,, \tag{1.3}$$

and τ_a denote Pauli matrices.

The low-energy regime of QCD is described by chiral perturbation theory [8]–[10] in terms of the dynamics of the pseudo-Goldstone bosons of broken chiral symmetry, which are the pions in our case. The pion fields $\pi_b(x)$ enter the SU(2)-valued matrices

$$U(x) = \exp\left(\frac{\mathrm{i}}{F_0}\,\pi_b(x)\tau_b\right), \tag{1.4}$$

which are the fundamental variables of chiral perturbation theory. The above representation in terms of pion fields refers to the vacuum $U = \mathbb{1}$ and is modified accordingly if the vacuum is at a different point. In leading order the chiral effective lagrangian including lattice effects up to $\mathcal{O}(a)$ is [11, 12]

$$\mathcal{L}_2 = \frac{F_0^2}{4}\,\mathrm{Tr}\left(\partial_\mu U^\dagger \partial_\mu U\right) - \frac{F_0^2}{4}\,\mathrm{Tr}\left(\chi U^\dagger + U\chi^\dagger\right) - \frac{F_0^2}{4}\,\mathrm{Tr}\left(\rho U^\dagger + U\rho^\dagger\right), \tag{1.5}$$

where

$$\chi = 2B_0(\tilde{m}\,\mathbb{1} - \mathrm{i}\,\mu\tau_3)\,, \tag{1.6}$$

appears in the chiral symmetry breaking mass term, and

$$\rho = 2W_0 a \mathbb{1} \tag{1.7}$$

parameterizes the lattice artifacts. The effective lagrangian in next to leading order including lattice artifacts up to order a^2 has been calculated by Bär, Rupak and Shoresh [13]. The introduction of a twisted mass term in chiral perturbation and its application to the calculation of pion masses and decay constants have been made in [12, 14].

The discussion of the phase diagram of lattice QCD in the framework of chiral perturbation theory has been pioneered by Sharpe and Singleton [15]. It is based on the potential contained in the chiral lagrangian. Let

$$U = u_0 \mathbb{1} + \mathrm{i}\, u_a \tau_a\,, \qquad a = 1, 2, 3\,, \tag{1.8}$$

so that

$$u \equiv (u_0, u_1, u_2, u_3) \tag{1.9}$$

is a unit 4-vector: $u \cdot u = 1$. The physical significance of the variable u_0 is given through its relation to the chiral condensate

$$\langle \bar{q}q \rangle = -2F_0^2 B_0 \langle u_0 \rangle \tag{1.10}$$

in leading order. The potential in next to leading order for the case of vanishing twist is of the form

$$V = -c_1\, u_0 + c_2\, u_0^2\,, \tag{1.11}$$

where

$$c_1 = 2F_0^2(B_0 m_q + W_0 a)\,. \tag{1.12}$$

Sharpe and Singleton discuss the region of quark masses, where they are small of order a^2, in which case both coefficients c_1 and c_2 are to be considered of order a^2.

In order to study the phase diagram in the $m_q - \mu$ plane the effect of the twisted mass term has to be incorporated. Its addition to the QCD lagrangian amounts to extend the potential to

$$V = -c_1\, u_0 + c_2\, u_0^2 + c_3\, u_3\,, \tag{1.13}$$

where

$$c_3 = 2F_0^2 B_0\, \mu\,. \tag{1.14}$$

As for the quark mass, the twist mass μ is also counted as being of order a^2, so that higher powers of μ are neglected for the moment.

Depending on the sign of c_2 there are now two possible scenarios for the phase structure, which will be discussed in the following.

2. Aoki scenario

We start by considering the case $c_2 > 0$, where an Aoki phase [16] appears. Let us first briefly recall the analysis of Sharpe and Singleton [15] for $\mu = 0$. If

$$|\epsilon| > 1\,, \qquad \text{where} \qquad \epsilon \equiv \frac{c_1}{2|c_2|}\,, \tag{2.1}$$

the potential has its minimum outside the allowed region $|u_0| \leq 1$ and consequently the vacuum is at $u_0 = 1, U = \mathbb{1}$ or at $u_0 = -1$, $U = -\mathbb{1}$, depending on the sign of c_1. The pion mass is given by

$$m_\pi^2 = \frac{1}{F_0^2}(|c_1| - 2c_2)\,. \tag{2.2}$$

Chiral symmetry $\mathrm{SU}(2)_L \otimes \mathrm{SU}(2)_R$ is broken explicitly to flavour $\mathrm{SU}(2)_V$.

On the other hand, for small quark masses, namely in the range

$$|\epsilon| < 1\,, \tag{2.3}$$

there is a small region of Aoki phase. The potential has its minimum at $u_0 = \epsilon$ and the remaining components of u develop a vacuum expectation value associated with spontaneous flavour and parity breaking, which can be chosen to be directed along the third axis: $u_3 = \pm\sqrt{1-\epsilon^2}$. The nonvanishing u_3 corresponds to

$$\langle \bar{\chi}\gamma_5\tau_3\chi \rangle \neq 0\,. \tag{2.4}$$

The remaining flavour symmetry is U(1) and π_1 and π_2 are the massless Goldstone bosons. The neutral pion is massive with a mass

$$m_{\pi 3}^2 = \frac{2c_2}{F_0^2}(1-\epsilon^2)\,. \tag{2.5}$$

Varying c_1 inside the Aoki phase from $\epsilon = 1$ to $\epsilon = -1$, the chiral condensate changes continuously from negative to positive values.

The boundary of the Aoki phase is at $|\epsilon| = 1$, where there is a second order phase transition and all pions are massless. The width of the phase is proportional to a^3.

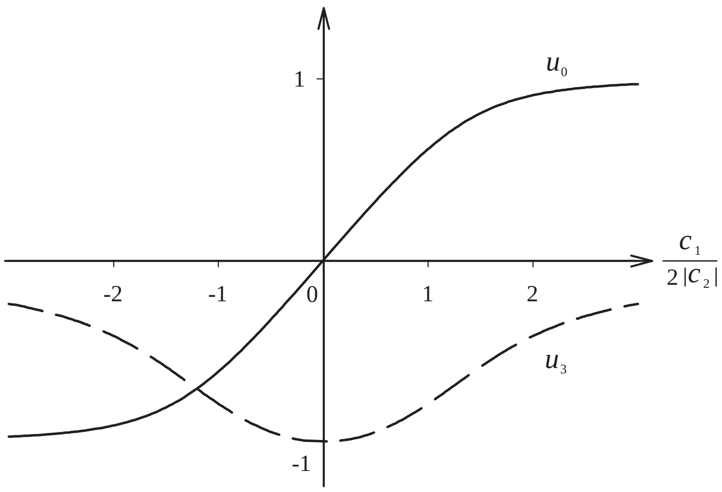

Figure 1: The values of u_0 and u_3 in the minimum of the potential as a function of $c_1/2|c_2| \propto \tilde{m}$ for $c_3 = c_2$ in the Aoki scenario. The curves represent the exact solutions to the quartic equations.

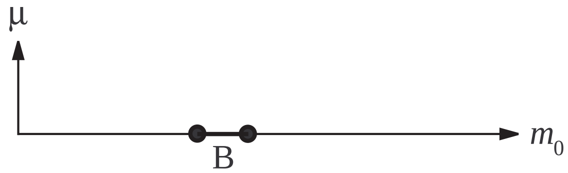

Figure 2: Phase diagram for the Aoki scenario.

Now let us switch on the twist mass to a nonvanishing value, which we may choose to be positive: $\mu > 0$. This leads to a shift of the minimum of the potential in the third direction. As a consequence, for all quark masses, u_3 acquires a nonvanishing negative value, which is given by the solution of a quartic equation and is shown in figure 1.

Instead of writing down the exact solution in terms of the formulae of Ludovico Ferrari [17] here, we restrict ourselves to displaying it to first order in $c_3 \propto \mu$ for $|\epsilon|$ away from 1:

$$u_3 = \begin{cases} -\dfrac{c_3}{|c_1| - 2c_2} + \mathcal{O}(c_3^2) \qquad \text{for} \quad |\epsilon| > 1\,, \\ -\sqrt{1-\epsilon^2} - \dfrac{\epsilon^2}{1-\epsilon^2}\,\dfrac{c_3}{4c_2} + \mathcal{O}(c_3^2) \qquad \text{for} \quad |\epsilon| < 1\,. \end{cases} \tag{2.6}$$

The breaking of flavour SU(2) is in this case explicit, and in addition to π_3 also the charged pions π_1 and π_2 are massive.

u_0 changes continuously as a function of the quark mass and there is no phase transition. The phase transition, that existed for $\mu = 0$, is washed out for $\mu \neq 0$. The phase diagram is shown in figure 2. Between the second order endpoints is a line of first order transitions, where u_3 makes a jump when going from positive to negative values of μ.

3. Normal scenario

A different scenario results for $c_2 < 0$. The case of vanishing μ has been discussed by Sharpe and Singleton [15] too. For $\mu = 0$ the potential has its minimum at $u_0 = 1$ for $c_1 > 0$, i.e. for positive quark mass, and at $u_0 = -1$ for $c_1 < 0$. At $c_1 = 0$, corresponding to the quark mass being equal to m_c, there is a first order phase transition, where u_0 jumps from $+1$ to -1. The chiral condensate makes a jump of size $-4F_0^2 B_0$. The pion masses are nonzero and are given by

$$m_\pi^2 = \frac{1}{F_0^2}(|c_1| + 2|c_2|)\,. \tag{3.1}$$

For $\mu \neq 0$ the minimum of the potential is shifted away from $u_0 = \pm 1$ by the "magnetic field" μ. We have $|u_0| < 1$ and $u_3 \neq 0$. The corresponding flavour and parity symmetry breaking is explicit and the pions remain massive.

The values of u_0 and u_3 are again given by the solution of a quartic equation, and are shown in figure 3.

To first order in μ we have

$$u_3 = -\frac{c_3}{|c_1| + 2|c_2|} + \mathcal{O}(c_3^2) \tag{3.2}$$

$$|u_0| = 1 - \frac{c_3^2}{2(|c_1| + 2|c_2|)^2} + \mathcal{O}(c_3^3)\,. \tag{3.3}$$

At $c_1 = 0$ there is a first order phase transition, where u_0 changes sign discontinuously, as indicated in figure 4. The value of u_3 at the transition is

$$u_3 = -\frac{c_3}{2|c_2|}\,. \tag{3.4}$$

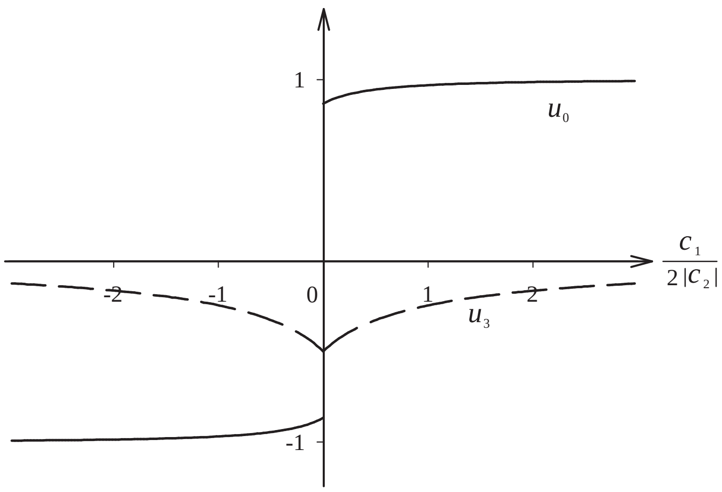

Figure 3: The values of u_0 and u_3 in the minimum of the potential as a function of $c_1/2|c_2| \propto \tilde{m}$ for $c_3 = |c_2|$ in the normal scenario. The curves represent the exact solutions to the quartic equations.

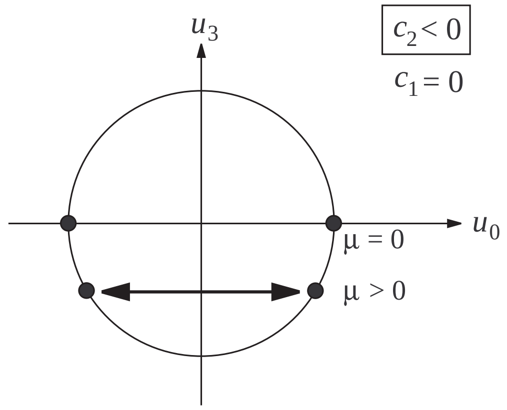

Figure 4: Jump of u_0 at the phase transition for the normal scenario.

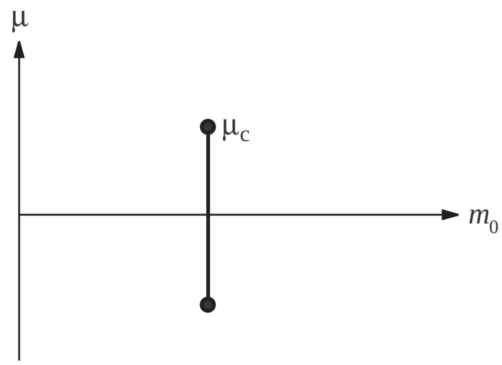

Figure 5: Phase diagram for the normal scenario.

For increasing μ the minima of the potential at the transition point $c_1 = 0$ approach each other. There is an endpoint of the transition line at

$$\mu_c = \frac{|c_2|}{F_0^2 B_0} \sim a^2 \tag{3.5}$$

and the phase diagram looks like it is shown in figure 5.

On the phase transition line the neutral pion mass behaves as

$$m_{\pi 3}^2 = \frac{1}{2F_0^2|c_2|}(4c_2^2 - c_3^2) \sim a^2 \tag{3.6}$$

and the same holds for the jump of the condensate,

$$\Delta\langle\bar{\chi}\chi\rangle = -4F_0^2 B_0 \sqrt{1 - \frac{c_3^2}{4c_2^2}} = -\frac{4F_0^3 B_0}{\sqrt{2|c_2|}} m_{\pi 3}\,, \tag{3.7}$$

as displayed in figure 6.

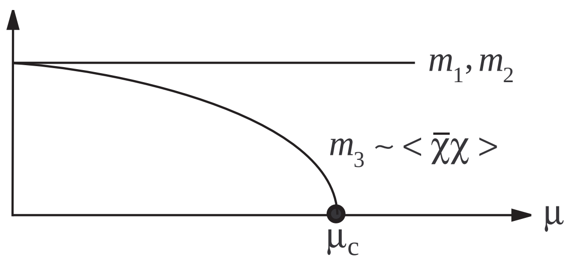

Figure 6: Pion masses and chiral condensate as a function of μ along the phase transition line in the normal scenario.

The masses of the charged pions are continuous across the first order line, where they have their minimum

$$m_{\pi 1}^2 = m_{\pi 2}^2 = \frac{2|c_2|}{F_0^2} \sim a^2 \,. \tag{3.8}$$

4. A new phase

So far we have considered the case of twist masses μ of order a^2 with only a linear term in u_3 in the potential. In general, higher terms in the Sharpe-Singleton potential have to be included. At the next order additional terms quadratic in u_a have to be added:

$$V = -c_1\, u_0 + c_2\, u_0^2 + c_3\, u_3 + c_4\, u_3^2 + c_5\, u_0 u_3 \,. \tag{4.1}$$

What are their possible consequences? In the normal scenario, $c_2 < 0$, one finds that these terms do not lead to qualitative changes of the phase diagram. Only numerical modifications will occur.

On the other hand, in the Aoki case the new terms can lead to new phases, if the coefficient $c_4 \propto \mu^2$ is positive. In this situation a minimum of the potential in the interior of the u_0–u_3 unit circle will occur for sufficiently large μ. As a consequence, flavour symmetry is broken down spontaneously to a discrete Z_2 by nonvanishing expectation values of u_1 or u_2. In addition to the segment of Aoki phase at $\mu = 0$, regions of this new phase in the upper ($\mu > 0$) or lower ($\mu < 0$) half-planes can form. Inside this phase the pion masses vanish and the quark condensate varies continuously.

Along the lines of catastrophe theory [18], terms in the potential of higher orders than quadratic do not change the discussed scenarios for small masses qualitatively as long as none of the quadratic coefficients above vanishes accidentally.

5. Discussion and conclusion

As we have seen, there can exist a line of first order phase transitions in the m_q–μ plane, terminating in second order endpoints. Depending on the sign of the coefficient c_2, the line is horizontal or vertical in the plane. Whereas for values of the inverse gauge coupling $\beta < 4.6$ the Aoki scenario appears to be realized [19], recent Monte Carlo calculations [5] at

$\beta = 5.2$ indicate the presence of the normal scenario. The first order phase transition line for nonvanishing μ occurs at a twist angle of $\pi/2$, where $\mathcal{O}(a)$ improvement is predicted [3, 4]. The associated two-phase coexistence and metastability hampers numerical calculations. Nevertheless, interesting physical observables, like decay constants and squared masses, are continuous across the phase transition line and are expected to be $\mathcal{O}(a)$ improved there.

From the point of view of Monte Carlo calculations it would be desirable to have the phase transition line as short as possible. There should be a value of β somewhere between 4.6 and 5.2 where $\mu_c \propto c_2$ vanishes. This point, however, would not be close enough to the continuum limit. In order to make μ_c small one could go nearer to the continuum limit at larger values of β, or try to improve the action in such a way that c_2 is small. One can search for such a situation on the untwisted axis ($\mu = 0$) by monitoring the minimum of the pion masses and trying to make it small. The jump of the condensate is not suitable for the search, as it is insensitive to c_2.

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References

[1] R. Frezzotti, P.A. Grassi, S. Sint and P. Weisz, *A local formulation of lattice QCD without unphysical fermion zero modes*, *Nucl. Phys.* **83** *(Proc. Suppl.)* (2000) 941 [hep-lat/9909003]; Alpha collaboration, R. Frezzotti, P.A. Grassi, S. Sint and P. Weisz, *Lattice QCD with a chirally twisted mass term*, *J. High Energy Phys.* **08** (2001) 058 [hep-lat/0101001].

[2] R. Frezzotti, *Wilson fermions with chirally twisted mass*, *Nucl. Phys.* **119** *(Proc. Suppl.)* (2003) 140 [hep-lat/0210007].

[3] R. Frezzotti and G.C. Rossi, *Chirally improving wilson fermions, 1. O(a) improvement*, *J. High Energy Phys.* **08** (2004) 007 [hep-lat/0306014].

[4] R. Frezzotti and G.C. Rossi, *Twisted mass lattice QCD with mass nondegenerate quarks*, *Nucl. Phys.* **128** *(Proc. Suppl.)* (2004) 193 [hep-lat/0311008].

[5] F. Farchioni et al., *Twisted mass quarks and the phase structure of lattice QCD*, hep-lat/0406039 and private communications.

[6] S.R. Sharpe and J.M.S. Wu, *The phase diagram of twisted mass lattice QCD*, hep-lat/0407025.

[7] S.R. Sharpe and J.M.S. Wu, *Applying chiral perturbation to twisted mass lattice QCD*, hep-lat/0407035.

[8] S. Weinberg, *Phenomenological lagrangians*, *Physica* **A96** (1979) 327.

[9] J. Gasser and H. Leutwyler, *Chiral perturbation theory to one loop*, *Ann. Phys. (NY)* **158** (1984) 142.

[10] J. Gasser and H. Leutwyler, *Chiral perturbation theory: expansions in the mass of the strange quark*, *Nucl. Phys.* **B 250** (1985) 465.

[11] G. Rupak and N. Shoresh, *Chiral perturbation theory for the Wilson lattice action*, *Phys. Rev.* **D 66** (2002) 054503 [hep-lat/0201019].

[12] G. Münster and C. Schmidt, *Chiral perturbation theory for lattice QCD with a twisted mass term*, *Europhys. Lett.* **66** (2004) 652 [hep-lat/0311032].

[13] O. Bär, G. Rupak and N. Shoresh, *Chiral perturbation theory at $O(a^2)$ for lattice QCD*, *Phys. Rev.* **D 70** (2004) 034508 [hep-lat/0306021].

[14] G. Münster, C. Schmidt and E.E. Scholz, *Chiral perturbation theory for partially quenched twisted mass lattice QCD*, hep-lat/0402003.

[15] S. Sharpe and R. Singleton, *Spontaneous flavor and parity breaking with Wilson fermions*, *Phys. Rev.* **D 58** (1998) 074501 [hep-lat/9804028].

[16] S. Aoki, *New phase structure for lattice QCD with Wilson fermions*, *Phys. Rev.* **D 30** (1984) 2653; *A solution to the* U(1) *problem on a lattice*, *Phys. Rev. Lett.* **57** (1986) 3136.

[17] in: G. Cardano, *Artis magnae sive de regulis algebraicis, Liber unus*, Joh. Petreium, Nürnberg, 1545.

[18] A. Held and P. Yodzis, *On the Einstein-Murphy interaction*, *Gen. Rel. Grav.* **13** (1981) 873.

[19] E.M. Ilgenfritz, W. Kerler, M. Müller-Preußker, A. Sternbeck and H. Stüben, *A numerical reinvestigation of the Aoki phase with $N_F = 2$ Wilson fermions at zero temperature*, *Phys. Rev.* **D 69** (2004) 074511 [hep-lat/0309057].

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