PHASE STRUCTURE OF LATTICE QCD
FOR GENERAL NUMBER OF FLAVORS

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We investigate the phase structure of lattice QCD for general number of flavors $N_F$. Based on numerical results combined with the result of the perturbation theory we propose the following picture: When $N_F \geq 17$, there is only a trivial fixed point and therefore the theory in the continuum limit is trivial. On the other hand, when $16 \geq N_F \geq 7$, there is a non-trivial fixed point and therefore the theory is non-trivial with anomalous dimensions, however, without quark confinement. Theories which satisfy both quark confinement and spontaneous chiral symmetry breaking in the continuum limit exist only for $N_F \leq 6$.

1 Introduction

The fundamental properties of QCD are quark confinement, asymptotic freedom and spontaneous breakdown of chiral symmetry. It is well-known that if the number of flavors exceeds $16\frac{1}{2}$, the asymptotic freedom is lost. Then, the question which naturally arises is whether there is constraint on the number of flavors for quark confinement and/or the spontaneous breakdown of chiral symmetry.

In our previous work, it was shown that in the strong coupling limit, when the number of flavors $N_F$ is greater than or equal to 7, quarks are deconfined and chiral symmetry is restored at zero temperature, if the quark mass is lighter than a critical value. In this work we investigate the problem of what is the condition on the number of flavors for quark confinement and spontaneous chiral symmetry breaking in the continuum limit.

As asymptotic freedom is the nature at short distance, one can apply the perturbation theory to investigate the critical number for it. However, because quark confinement and spontaneous chiral symmetry breaking are due to non-perturbative effects, one has to apply a non-perturbative method throughout the investigation of the critical numbers for them. Therefore we employ lattice QCD for the study in this work, since lattice QCD is such a theory constructed non-perturbatively.

In order to investigate the condition on the number of flavors $N_F$ in the continuum limit, we first clarify the phase structure at zero temperature for general number of flavors, in particular, for $N_F \geq 7$. When the phase diagram becomes clear, we are able to see what kind of continuum limit exists and
eventually answer the question given above.

In Sec. 2 the formulation of lattice QCD is introduced. The notations which will be used later, and the Wilson quark action and the standard one-plaquette gauge action which we employ in this work are given. In Sec. 3 quark mass is defined and chiral property in the Wilson formalism of fermions is discussed. Before going into details a brief summary is given Sec. 4. In Secs. 5 - 10, details of numerical simulations and results are given. Conclusions are given in Sec. 11.

2 Lattice QCD

Lattice QCD is defined on a hypercubic lattice in 4-dimensional euclidean space with lattice spacing $a$. A site is denoted by a vector $n = (n_1, n_2, n_3, n_4)$, where $n_i$'s are integers. A link with end points at the sites $n$ and $n + \hat{\mu}$ is specified by a pair $(n, \mu)$, where $\hat{\mu}$ denotes a unit vector in the $\mu$ direction.

The gauge variable $U_{n,\mu}$ which is an element of SU(3) gauge group is defined on the link $(n, \mu)$. The action for gluons which we adopt is given by

$$S_{gauge} = \frac{1}{g^2} \sum_{n, \mu \neq \nu} \text{Tr}(U_{n,\mu}U_{n+\hat{\mu},\nu}U_{n+\hat{\nu}+\hat{\mu},\mu}U_{n+\hat{\nu},\nu}^\dagger),$$

where $g$ is the gauge coupling constant. This action is called the standard one-plaquette gauge action. We usually use, instead of the bare gauge coupling constant $g$, $\beta$ defined by

$$\beta = \frac{6}{g^2}.$$

The quark variable is a Grassman number defined at a site. It is well-known that a naive discretization of the Dirac action

$$S_{fermion} = \frac{a^3}{2} \sum_{n, \mu} (\bar{q}_n \gamma_\mu q_{n+\hat{\mu}} - \bar{\tilde{q}}_{n+\hat{\mu}} \gamma_\mu q_n) + m_0 a^4 \sum_n \bar{q}_n q_n,$$

with $m_0$ being the bare fermion mass, leads to 16 poles instead of one pole. This problem is called the species doubling. To avoid this problem K. Wilson proposed adding to the naive discretized action a dimension 5 operator called the Wilson term

$$-a^3 \sum_{n, \mu} (\bar{q}_n q_{n+\hat{\mu}} - 2\bar{\tilde{q}}_n q_n + \bar{\tilde{q}}_{n+\hat{\mu}} q_n),$$

with $\bar{\tilde{q}}_n$ defined by

$$\bar{\tilde{q}}_n = \sum_{\mu} \bar{q}_n \gamma_\mu q_{n+\hat{\mu}}.$$
Rescaling the fermion field by $q = \sqrt{2K}\psi$ and making the action gauge invariant, we obtain the Wilson fermion action

$$S_{\text{Wilson}} = a^3 \sum_n [\bar{\psi}_n \psi_n - K \{\bar{\psi}_n (1 - \gamma_\mu) U_{n,\mu} \psi_{n+\hat{\mu}} + \bar{\psi}_{n+\hat{\mu}} (1 + \gamma_\mu) U_{n,\mu}^\dagger \psi_n\}].$$

(5)

where

$$K = \frac{1}{(m_0 a + 4r)},$$

(6)

which is called the hopping parameter.

The full action $S$ is given by the sum of the gauge part $S_{\text{gauge}}$ and the fermion part $S_{\text{Wilson}}$,

$$S = S_{\text{gauge}} + S_{\text{Wilson}}.$$  

(7)

The expectation value of an operator $\mathcal{O}(U, \psi, \bar{\psi})$ is given by

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_{n,\mu} dU_{n,\mu} \prod_n d\psi_n d\bar{\psi}_n \mathcal{O}(U, \psi, \bar{\psi}) \exp(S),$$

(8)

where $Z$ is the partition function

$$Z = \int \prod_{n,\mu} dU_{n,\mu} \prod_n d\psi_n d\bar{\psi}_n \exp(S),$$

(9)

with $dU_{n,\mu}$ being the Haar measure of SU(3).

In the case of degenerate $N_F$ flavors, lattice QCD contains two parameters: the gauge coupling constant $\beta = 6/g^2$ and the hopping parameter $K$. In the non-degenerate case, the number of the hopping parameters is $N_F$.

The lattice spacing $a$ is a function of the bare coupling constant which is defined through the RG beta function. The continuum limit is the limit where the lattice spacing $a$ goes to zero in such a way that physical quantities are kept constant. In an asymptotically free case the limit corresponds to the limit where the coupling constant $g$ vanishes.

At finite temperatures the linear extension in the time direction $N_t$ is much smaller that those in the spatial directions $(N_x, N_y, N_z)$. The temperature $T$ is given by

$$1/N_t a.$$ 

For gluons the periodic boundary condition is imposed, while for quarks an anti-periodic boundary condition is imposed in the time direction.
3 Quark mass and chiral symmetry in the Wilson quark action

In the formalism of Wilson of quarks on the lattice, the flavor symmetry as well as C, P and T symmetries are exactly satisfied on a lattice with a finite lattice spacing. However, chiral symmetry is explicitly broken by the Wilson term even for the vanishing bare quark mass \( m_0 = 0 \). The lack of chiral symmetry causes much conceptual and technical difficulties in numerical simulations and physics interpretation of data. (See for more details Ref. and references cited there.)

The chiral property of the Wilson fermion action was first systematically investigated through Ward identities by Bochicchio et al. We also independently proposed to define the current quark mass by

\[
2m_q < 0 \mid P \mid \pi > = -m_\pi < 0 \mid A_4 \mid \pi >
\]

where \( P \) is the pseudoscalar density and \( A_4 \) the fourth component of the local axial vector current. We use this definition of the current quark mass in this work. In general we need a multiplicative normalization factor for the axial current, which we have absorbed into the definition of the quark mass, because this definition is sufficient for later use. The value of the quark mass does not depend on whether the system is in the high or the low temperature phase when the gauge coupling constant is not so large: \( \beta \geq 5.5 \) for \( N_F = 2 \).

With this definition of quark mass, the pion mass vanishes in the chiral limit where the quark mass vanishes at zero temperature, for \( N_F \leq 6 \). However, in the deconfining phase at finite temperatures the pion mass does not vanish in the chiral limit. It is almost equal to twice the lowest Matsubara frequency \( \pi/N_t \). This implies that the pion state is a free two-quark state. Quarks are not confined. The pion mass is nearly equal to the scalar meson mass, and the rho meson mass to the axial vector meson mass. The chiral symmetry is also manifest within corrections due to finite lattice spacing.

Thus hadron masses in the chiral limit where the current quark mass vanishes clarifies the phase of the system at finite temperatures for \( N_F \leq 6 \). We use the same strategy to discriminate the phase of QCD with various number of flavors \( N_F \): the pion mass at zero quark mass determines whether chiral symmetry is spontaneously broken or not, and also whether quarks are confined or not. It should be noted that in QCD with \( N_F \) flavors there is no known order parameter for quark confinement. When the pion mass is about twice the lowest Matsubara frequency we conclude that quarks are not confined.
4 Brief Summary

Before going into details let me give a brief summary, because the following sections will be too technical for non-experts of lattice QCD.

In Fig. 1 is presented our conjecture in terms of the beta function of renormalization group. Here $g$ is the bare gauge coupling constant. When $N_F$ is equal or smaller than 6, the beta function is negative for all coupling constants. On the other hand, when $N_F$ is equal or larger than 17, it is positive. In the case when $N_F$ is between 7 and 16, it changes sign from negative to positive with increasing $g$. Therefore there is a non-trivial IR fixed point. The existence of such a fixed point was first pointed out by Banks and Zaks. However, our picture is different those proposed by them. Fig. 2 is the conjecture made by Banks and Zaks. They assumed that the beta function becomes negative for large enough coupling constant for all $N_F$. This point is different from ours. Their critical value is 9, which is also different from our value 7.

It is sometimes argued in the literature that quarks are confined in the strong coupling constant. Although there is a proof for quark confinement in the strong coupling constant in the pure $SU(3)$ gauge theory, there are no
such proofs in QCD with dynamical quarks. Our previous result \[N_F < N'\] is a counter example for such an argument.

Fig. 3 shows the phase structure in the $\beta$ - $K$ plane for various number of flavors. When $N_F \leq 6$, there is the chiral limit $K_c(\beta)$, where the current quark mass $m_q$ vanishes, in the confining phase. The value of $K_c(\beta)$ at $\beta = \infty$ is $1/8$, which corresponds to the vanishing bare quark mass $m_0 = 0$. As $\beta$ decreases, the $K_c$ increases, up to $1/4$ at $\beta = 0$. If the action would be chiral symmetric, the chiral line should be a constant, $1/8$. The line $K = 0$ corresponds to an infinite quark mass. Quarks are confined for any value of the current quark mass for all values of $\beta$.

When $N_F \geq 7$, there is no chiral limit in the confining phase. There is a line of a first order phase transition from the confining phase to a deconfining phase at a finite current quark mass for all values of $\beta$. It is crucial that the point $K = 1/8$ at $\beta = \infty$ does belong to a deconfining phase. The chiral line which starts from this point hits the boundary between the confining phase and the deconfining phase at finite $\beta$ as shown in Fig. 3 for the case where $N_F$ is not too large. This situation makes the interpretation of numerical data difficult; the data around $\beta = 4.5$ for $N_F = 7, 12$ and 18 look very complicated.
In order to understand the structure of the deconfining phase more clearly, we increase $N_F$ up to 300, because the region of the deconfining phase becomes larger with larger $N_F$, and consequently the structure becomes simple, as shown in Fig. 3. When $N_F \geq 240$, the chiral line where the quark mass vanishes goes straight from $\beta = \infty$ to $\beta = 0$, without hitting the phase transition boundary. We have made a MCRG study to investigate the flow of RG along the massless line. The direction at $\beta = \infty$ is known from the perturbation theory, from left to right in the $\beta$ - $K$ plane. Our results of a MCRG study which will be described later implies that the direction is identical all through the $\beta$ region. Thus there is only a trivial IR fixed point at $\beta = \infty$. There are no other fixed points where we are able to take a continuum limit of the theory with quarks. Thus the theory is a trivial free theory.

As $N_F$ decreases, the massless quark line hits the boundary of a first order phase transition. Except this point other general features are the same as
those for $N_F \geq 240$. Massless quarks exist only in the deconfining phase. A continuum limit can be taken only at a fixed point on this line. Although we have not investigated the flow of RG, we naturally assume that the direction for $N_F \leq 17$ is the same as that for $N_F \geq 240$. Thus the theory is also trivial for $N_F \leq 17$.

When $7 \leq N_F \leq 16$, the phase structure seems to be not too much different from those for $N_F \geq 17$. However, the flow of RG at $\beta = \infty$ is opposite to that for $N_F \geq 17$, because the theory is asymptotically free. Therefore a continuum limit is governed by an IR fixed point which should exist somewhere at finite value of $\beta$. Unfortunately, as explained above, the massless line hits the boundary in the two parameter space. Therefore it is hard to see numerically where the IR fixed point exists. When one makes a RG transformation the trajectory moves into, in general, a multi-parameter space. Thus within the two parameter space we are investigating here it is difficult to pin down the position of the IR fixed point. However, even without knowing the position we are able to discuss the nature of the continuum limit. On the massless line around $\beta = 4.5$, the mass of the pion is roughly twice the lowest Matsubara frequency. This implies that the quark is almost free. That is, an anomalous
dimension which is governed by the IR fixed point is small. The fact that the anomalous dimension is small suggests that the IR fixed point exists at finite $\beta$.

If the IR fixed point would exist at $\beta = 0$ or $g = \infty$, the anomalous dimension would be large or infinite. Anyway, the fact that the mass of the pion is roughly twice the lowest Matsubara frequency implies that quarks are not confined in this phase and the chiral symmetry is not spontaneously broken. Thus this phase is a phase governed by a non-trivial IR fixed point.

A salient fact for the above in this section is that in the strong coupling limit, when the number of flavors $N_F$ is greater than or equal to 7, quarks are deconfined and chiral symmetry is not spontaneously broken at zero temperature, if the quark mass is lighter than a critical value, which was shown in our previous work.

In the following sections details of numerical simulations will be given. One has to perform numerical simulations on a lattice with a finite $N_t$. This implies that when $\beta$ becomes large one encounters a finite temperature phase transition. A schematic diagram is shown in Fig. 4 for the case $N_F \leq 6$. In the case $N_F \geq 7$, one has to be careful about the existence of both zero temperature transitions and finite temperature transitions.

5 Simulation parameters

The lattice sizes are $8^2 \times 10 \times N_t$ ($N_t = 4$, 6 or 8), $16^2 \times 24 \times N_t$ ($N_t = 16$) and $18^2 \times 24 \times N_t$ ($N_t = 18$). We use an anti-periodic boundary condition for quarks in the $t$ direction and periodic boundary conditions otherwise. When the hadron spectrum is calculated, the lattice is duplicated in the direction of lattice size 10 for $N_t \leq 8$, which we call the $z$ direction. We call the pion screening mass simply the pion mass and similarly for the quark mass.

We use the hybrid R algorithm for the gauge configuration generation. As $N_F$ increases we have to decrease $\Delta \tau$, such as $\Delta \tau = 0.0025$ for $N_F = 240$, to reduce $O(\Delta \tau^2)$ errors. We have checked that the errors are sufficiently small selecting typical cases.

6 $K_d$ versus $N_F$

We first study the case of $\beta = 0$ as in the previous work. Fig. 3a shows the results of the deconfining transition points $K_d$ at $\beta = 0$ obtained on $N_t = 4$ lattices for various numbers of $N_F$ (see also Fig. 1).

The data of plaquette for $N_F = 240$ at $\beta = 0$ indicates that the deconfining transition is of first order and that the location of the transition point is independent of $N_t$ for large $N_t$ ($1/K_d \simeq 8.1$ for $N_t = 4$ and $1/K_d \simeq 7.75$ for $N_t = 8$ and 16). Therefore we conclude that the transition is bulk as is
Figure 5: a) The transition point $1/K_d$ at $\beta = 0$ versus $N_F$ at $N_t = 4$ and $N_t \geq 8$. For clarity, data at $N_t = 8$ for $N_F = 300$ is slightly shifted in the figure. Shaded region was investigated in our previous study. b) Plaquette versus $1/K$ at $\beta = 0$ for various number of $N_F$ at $N_t = 4$.

confirmed in our previous work for $N_F = 7$. In Fig. 5a, the transition points at $N_t \geq 8$ for $N_F = 7$, 240 and 300 are also included. These values are roughly those for the bulk transition points at zero temperature.

As $N_F$ increases up to 240, $1/K_d$ approaches toward or exceeds the value 8, which is the value of $1/K$ for a massless free quark. Because of this, for $N_F \gtrsim 240$, we are able to see a wide region of the deconfining phase in the whole range of $\beta$. Therefore we intensively investigate the case $N_F = 240$, and then decrease $N_F$. 

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7 $N_F = 240$

Fig. 6 shows the results of $m_{\pi}^2$ and $2m_q$ for $N_F = 240$ at $\beta = 0, 2.0, 4.5, 6.0,$ and $100$ on the $N_t = 4$ lattice. A very striking fact is that the shape of $m_{\pi}^2$ and $2m_q$ as a function of $1/K$ only slightly changes for $1/K < 8$ when the value of $\beta$ decreases from $\infty$ down $0$. (Note that the values at $\beta = \infty$ are those for free quarks.) Only the position of the local minimum of $m_{\pi}^2$ at $1/K \approx 8$, which corresponds to the vanishing point of $m_q$, slightly shifts toward smaller $1/K$. We obtain similar results also for $N_t = 8$.

From these data we propose the phase diagram in Fig. 7 for $N_F = 240$. The dark shaded line is the phase boundary between the confining phase and the deconfining phase at zero temperature. When $N_t = 4$ or $8$, the boundary line bends down at finite $\beta$ as shown in Fig. 7 due to the finite temperature phase transition of the confining phase.

The dashed line corresponds to the $m_q = 0$ line. This line also corresponds to the minimum point of $m_{\pi}^2$. We have also calculated the quark propagator in the Landau gauge and checked that chiral symmetry of the propagator, $\gamma_5 G(z) \gamma_5 = -G(z)$, is actually satisfied on the $m_q = 0$ line.

The results for the case $N_F = 300$ are essentially the same as those for $N_F = 240$ except for very small shifts of the transition point and the minimum point of $m_{\pi}^2$. 

Figure 6: $m_{\pi}^2$ and $2m_q$ versus $1/K$ for $N_F = 240$ at $N_t = 4$. 
8 Renormalization group flow

The $m_q = 0$ point at $\beta = \infty$ is the trivial IR fixed point for $N_F \geq 17$. The phase diagram shown in Fig. 7 suggests that there are no other fixed points on the $m_q = 0$ line at finite $\beta$.

In order to confirm this, we investigate the direction of Renormalization Group (RG) flow along the $m_q = 0$ line for $N_F = 240$, using a Monte Carlo Renormalization Group (MCRG) method.

One problem here is that it is practically impossible to make simulations in the massless limit at zero temperature due to the existence of zero modes in the quark matrix. Therefore, we impose an anti-periodic boundary condition in the $t$ direction.

We make a block transformation for a change of scale factor 2, and estimate the quantity $\Delta \beta$ for the change of $a \to a' = 2a$. We generate configurations on an $8^4$ lattice on the $m_q = 0$ points at $\beta = 0$ and 6.0 and make twice blockings. We also generate configurations on a $4^4$ lattice and make once a blocking. Then we calculate $\Delta \beta$ by matching the value of the plaquette at each step.

From the matching, we obtain $\Delta \beta \simeq 6.5$ for $\beta = 0$ and 10.5 for $\beta = 6.0$. The value obtained from the perturbation theory is $\Delta \beta \simeq 8.8$ at $\beta = 6.0$ for $N_F = 240$. The signs are the same and the magnitudes are comparable. This suggests that the directions of RG flow on the $m_q = 0$ line at $\beta = 0$ and 6.0 are the same as that at $\beta = \infty$ for $N_F = 240$. This further suggests that there are no fixed points at finite $\beta$. All of the above imply that the theory is trivial.

$^a$ It is known for the pure $SU(3)$ gauge theory, in particular in the deconfining phase, that one has to make a more careful analysis using several types of Wilson loop to extract a precise value of $\Delta \beta$. We reserve elaboration of this point and a fine tuning of $1/K$ at each $\beta$ for future works.
in the case of $N_F = 240$.

\[9\] $240 \geq N_F \geq 17$

Now we decrease the value of $N_F$ from 240. When $\beta = 6.0$, the shapes of $m_\pi^2$ are almost identical to each other, except for a slight shift toward smaller $1/K$ as $N_F$ decreases.

When $\beta = 0$, the boundary of the first order phase transition between the deconfining phase and the confining phase moves toward smaller $1/K$ and therefore the range of the deconfining phase decreases: $1/K_d \approx 8.5$, 8, 7.6, 7.2, 6.1 for $N_F = 300$, 240, 180, 120 and 60, respectively, as shown in Fig. 8. For $N_F = 18$, the value of $1/K_d$ decreases down to 5.0.

Due to the fact that the confining phase invades the deconfining phase, the massless line in the deconfining phase hits the boundary at finite $\beta$ when $N_F$ becomes small. For example, in the case of $N_F = 18$, as shown in Fig. 8, it hits at $\beta = 4.0 - 4.5$.

Although the area of the deconfining phase decreases with decreasing $N_F$, the shape and the position of $m_\pi^2$ in the part of deconfining phase only slightly change from $N_F = 300$ to 18. The values of $m_q$ as functions of $1/K$ also show only slight changes in the deconfining phase. These facts, combined with the perturbative result that for $N_F \geq 17$, $\beta = \infty$ is the IR fixed point, suggest that the RG flow along the massless quark in the deconfining phase is the same as that for $N_F = 240$. In this case, the theory is trivial for $N_F \geq 17$.

\[b\] Although we have investigated only down to the $N_F = 18$ case, we do not expect any qualitative differences between the cases of $N_F = 17$ and 18.

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When \( N_F \leq 16 \), the theory is asymptotic free. On the other hand, quark confinement is lost for \( N_F \geq 7 \) even in the strong coupling limit \( \beta = 0 \). Therefore the question is what happens for the cases \( 16 \geq N_F \geq 7 \) in the continuum limit.

We have intensively simulated the cases \( N_F = 12 \) and 7. The phase diagram for \( N_F = 12 \) is shown in Fig. 9. Although the gross feature of the phase diagram seems to be not too much different from the case of \( N_F = 18 \) which is shown in Fig. 8, the flow of RG at \( \beta = \infty \) is opposite to that for \( N_F \geq 17 \), because the theory is asymptotically free. Therefore a continuum limit is governed by an IR fixed point which should exist somewhere at finite value of \( \beta \). Unfortunately, as explained above, the massless line hits the boundary in the two parameter space. Therefore it is hard to see numerically where the IR fixed point exists. When one makes a RG transformation the trajectory moves into, in general, a multi-parameter space. Thus within the two parameter space we are investigating here it is difficult to pin down the position of the IR fixed point. Even without knowing the position we are able to discuss the nature of the continuum limit. On the massless line around \( \beta = 4.5 \), the mass of the pion is roughly twice the lowest Matsubara frequency. This implies that the quark is almost free. That is an anomalous dimension which is governed by the IR fixed point is small. The fact that the anomalous dimension is small suggests that the IR fixed point exists at finite \( \beta \): If the IR fixed point would exist at \( \beta = 0 \) or \( g = \infty \), the anomalous dimension would be large or infinite. Anyway, the fact that the mass of the pion is roughly twice the lowest Matsubara frequency implies that quarks are not confined in this phase and the chiral symmetry is not spontaneously broken. Thus this
phase is a phase governed by a non-trivial IR fixed point. The theory in the continuum limit is a non-trivial theory with anomalous dimensions, however, without confinement. We reserve for future works a detailed RG study to find a non-trivial fixed point in a wider parameter space.

11 Conclusions

Based on numerical results combined with the result of the perturbation theory we propose the following picture: There are three categories depending on the number of flavors $N_F$: a free theory for $N_F \geq 17$, a non-trivial theory governed by a non-trivial IR fixed point for $16 \geq N_F \geq 7$ and confinement and spontaneous chiral symmetry breaking for $N_F \leq 6$.

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